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APPLICATION

for

UNITED STATES LETTERS PATENT

on

1,2-DISUBSTITUTED-6-OXO-3-PHENYL-PIPERIDINE-3-CARBOXAMIDES
AND COMBINATORIAL LIBRARIES THEREOF

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1,2-DISUBSTITUTED-6-OXO-3-PHENYL-PIPERIDINE-3-CARBOXAMIDES.

AND COMBINATORIAL LIBRARIES THEREOF

FIELD OF THE INVENTION

[0001] The present invention relates generally to the synthesis of compounds comprising piperidine-3-carboxamides. In one embodiment, the invention provides novel 1,2-disubstituted-6-oxo-3-phenyl-piperidine-3-carboxamide derivative compounds as well as novel combinatorial libraries comprised of such compounds.

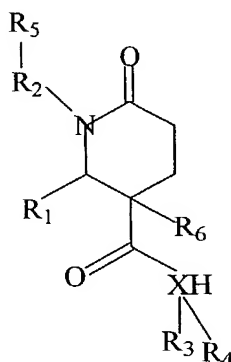
BACKGROUND INFORMATION

[0002] The process of discovering new therapeutically active compounds for a given indication involves the screening of all compounds from available compound collections. From the compounds tested, one or more structures are selected as a promising lead. A large number of related analogs are then synthesized in order to develop a structure-activity relationship and select one or more optimal compounds. With traditional "one-at-a-time" synthesis and biological testing of analogs, this optimization process is long and labor intensive. Adding significant numbers of new structures to the compound collections used in the initial screening step of the discovery and optimization process cannot be accomplished with traditional "one-at-a-time" synthesis methods, except over a time frame of years or even decades. Faster methods are needed that allow for the preparation of up to thousands of related compounds in a matter of days or a few weeks. This need is particularly evident when it comes to synthesizing more complex compounds, such as piperidine-3-carboxamide derivative compounds.

[0003] Combinatorial approaches have been extended to "organic," or non-peptide, libraries. However, the libraries to date contain compounds of limited

SUMMARY OF THE INVENTION

[0006] The present invention relates to novel piperidine-3-carboxamide derivative compounds of the following formula:



wherein

[0007] X is selected from the group consisting of N and O;

[0008] R₁ is selected from the group consisting of a substituted aromatic heterocyclic ring, C₃-C₁₂ substituted alicycle and substituted phenyl;

[0009] R₂ is selected from the group consisting of H; -OH; C₁ to C₇ alkoxy; C₁ to C₇ substituted alkoxy; C₂-C₇ alkenyl; C₁ to C₇ substituted alkenyl; C₂ to C₇ alkynyl; C₂ to C₇ substituted alkynyl; unsubstituted phenyl; naphthyl; substituted phenoxy; C₂ to C₇ heterocyclic ring; substituted C₂ to C₇ heterocyclic ring; substituted cyclic C₂ to C₇ alkylene; C₁ to C₇ alkyl; C₁ to C₇ substituted alkyl; C₃ to C₇ cycloalkyl; C₃ to C₇ substituted cycloalkyl; C₁ to C₇ alkoxy; halo; C₁ to C₁₀ alkylthio; C₁ to C₁₀ substituted alkylthio; C₁ to C₁₀ alkyl nitrile; a C₇ to C₁₈ substituted phenylalkyl; substituted phenyl;

[0010] R₃ and R₄ are independently selected from the group consisting of -OH; H; C₁ to C₆ alkyl; C₁ to C₇ substituted alkyl; C₂ to C₇ alkenyl; C₁ to C₇ alkoxy; C₁ to C₇ substituted alkoxy; C₃ to C₇ cycloalkyl; C₃ to C₇ substituted cycloalkyl; C₁

to C₁₀ alkylthio; C₁ to C₁₀ alkynitrile; C₁ to C₄ alcohol; substituted phenyl; C₁ to C₆ substituted alkyl; C₁ to C₇ alkoxy; C₃ to C₇ cycloalkyl; and C₃ to C₇ substituted cycloalkyl; C₂ to C₇ heterocyclic ring; C₂ to C₇ substituted heterocyclic ring; phenoxy; and substituted phenoxy,

[0011] R₅ is selected from the group consisting of H and NH₂, and

[0012] R₆ is selected from the group consisting of phenyl, substituted phenyl, C₂ to C₇ heterocyclic ring, and substituted C₂ to C₇ heterocyclic ring.

[0013] The invention further relates to combinatorial libraries containing two or more such compounds, as well as methods of preparing piperidine-3-carboxamide derivative compounds.

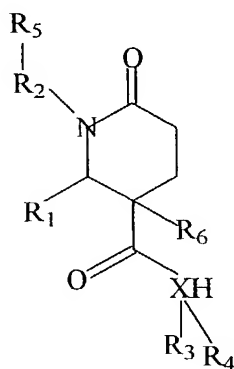
BRIEF DESCRIPTION OF THE DRAWING

[0014] Figures 1 and 2 show two parts of a scheme for the combinatorial synthesis of piperidine-3-carboxamide derivative compounds.

[0015] Figure 3 shows a scheme for the production of (Substituted Phenyl)-glutaric anhydrides.

DETAILED DESCRIPTION OF THE INVENTION

[0016] The present invention provides compounds and combinatorial libraries of compounds of the formula:



wherein:

[0017] X is selected from the group consisting of N and O;

[0018] R₁ is selected from the group consisting of a substituted aromatic heterocyclic ring, C₃-C₁₂ substituted alicycle and substituted phenyl;

[0019] R₂ is selected from the group consisting of H; -OH; C₁ to C₇ alkoxy; C₁ to C₇ substituted alkoxy; C₂-C₇ alkenyl; C₁ to C₇ substituted alkenyl; C₂ to C₇ alkynyl; C₂ to C₇ substituted alkynyl; unsubstituted phenyl; naphthyl; substituted phenoxy; C₂ to C₇ heterocyclic ring; substituted C₂ to C₇ heterocyclic ring; substituted cyclic C₂ to C₇ alkylene; C₁ to C₇ alkyl; C₁ to C₇ substituted alkyl; C₃ to C₇ cycloalkyl; C₃ to C₇ substituted cycloalkyl; C₁ to C₇ alkoxy; halo; C₁ to C₁₀ alkylthio; C₁ to C₁₀ substituted alkylthio; C₁ to C₁₀ alkyl nitrile; a C₇ to C₁₈ substituted phenylalkyl; substituted phenyl;

[0020] R₃ and R₄ are independently selected from the group consisting of -OH; H; C₁ to C₆ alkyl; C₁ to C₇ substituted alkyl; C₂ to C₇ alkenyl; C₁ to C₇ alkoxy; C₁ to C₇ substituted alkoxy; C₃ to C₇ cycloalkyl; C₃ to C₇ substituted cycloalkyl; C₁ to C₁₀ alkylthio; C₁ to C₁₀ alkyl nitrile; C₁ to C₄ alcohol; substituted phenyl; C₁ to C₆ substituted alkyl; C₁ to C₇ alkoxy; C₃ to C₇ cycloalkyl; and C₃ to C₇ substituted cycloalkyl; C₂ to C₇ heterocyclic ring; C₂ to C₇ substituted heterocyclic ring; phenoxy; and substituted phenoxy,

[0021] R₅ is selected from the group consisting of H and NH₂, and

[0022] R₆ is selected from the group consisting of phenyl, substituted phenyl, C₂ to C₇ heterocyclic ring, and substituted C₂ to C₇ heterocyclic ring.

[0023] The invention also provides methods of preparing piperidine-3-carboxamide derivative compounds and combinatorial libraries. In one method, as shown in Figures 1 and 2, such compounds can be prepared by a process comprising:

[0024] preparing a resin bound aldehyde or diamine,

[0025] reacting said resin bound aldehyde with an amine, or said resin bound diamine with an aldehyde, to form a resin bound imine,

[0026] cyclizing said resin bound imine to produce a resin bound carboxylic acid,

[0027] acylating said resin bound carboxylic acid, and

[0028] cleaving and extracting said piperidine-3-carboxamide derivative compound from said resin.

[0029] Examples of aldehydes which are useful in the above reaction include but are not limited to 4-hydroxybenzaldehyde, 3-hydroxybenzaldehyde, 2-hydroxy-5-methylbenzaldehyde, 3,5-dimethyl-4-hydroxybenzaldehyde, 2-hydroxy-4-methoxybenzaldehyde, 3-ethoxysalicylaldehyde, 2-hydroxy-1-naphthaldehyde, 5-bromosalicylaldehyde, cyclopropanecarboxaldehyde, 3-furaldehyde, benzaldehyde, 2-thiophenecarboxaldehyde, 3-thiophenecarboxaldehyde, P-tolualdehyde, 4,5-dimethyl-2-furancarboxaldehyde, P-anisaldehyde, 5-methylfurfural, O-tolualdehyde, 2,4,5-trimethylbenzaldehyde, piperonal, 5-methyl-2-thiophenecarboxaldehyde, 4-(difluoromethoxy)benzaldehyde, 5-bromo-2-furaldehyde, 4-biphenylcarboxaldehyde and 5-bromo-2-thiophenecarboxaldehyde.

[0030] Examples of diamines and amines useful in the above reaction when producing a resin bound diamine or reaction an aldehyde with an amine, include but are not limited to methylamine, ethylamine, propargylamine, cyclopropylamine, allylamine, propylamine, 3-aminopropionitrile, isobutylamine, cyclopentylamine, cyclohexylamine, hexylamine, N-acetylenediamine, 3-ethoxypropylamine, 4-chlorobenzylamine, 1-(3-aminopropyl)-2-pyrrolidinone, tryptamine, 3-(trifluoromethyl)benzylamine, 2,4-dichlorophenethylamine, 4-amino-1-benzylpiperidine, benzylamine, ethylenediamine, 1,3-diaminopropane, 1,4-diaminobutane, trans-1,2-cyclohexanediamine, trans-1,4-diaminocyclohexane, 2,2-thiobis(ethylamine), and N,N-Bis(3-aminopropyl)methylamine.

[0031] Examples of amines useful in the above reaction when acylating the resin bound carboxylic acid include but are not limited to nipecotamide, 1-(2-aminoethyl)pyrrolidine, pyrrolidine, histamine, cyclopentylamine, allylamine, 2-methoxyethylamine, cyclohexylamine, 1-methylpiperazine, tetrahydrofurfurylamine, 4-methylbenzylamine, 3-fluorobenzylamine, 4-fluorobenzylamine, 1-(3-aminopropyl)imidazole, cyclopropylamine, propylamine, ethanolamine, 2-thiophenemethylamine, n,n-dimethyl-1,3-propanediamine, 1-(2-

aminoethyl)piperidine, isoamylamine, 3-ethoxypropylamine, (r)-(-)-1-cyclohexylethylamine, neopentylamine, 3-(methylthio)propylamine, isobutylamine, 3-amino-1-propanol, 2-ethoxyethylamine, 2,6-dimethylpiperazine, propargylamine, thiophene-2-ethylamine, butylamine, 2-amino-1-methoxypropane, 3-aminopropionitrile, 3-methylpiperidine, P-anisidine, 1,2,3,6-tetrahydropyridine, 2,6-dimethylmorpholine, methoxyamine hydrochloride, n-ethylpiperazine, water, and hydroxylamine.

[0032] When the above-described compounds include one or more chiral centers, the stereochemistry of such chiral centers can independently be in the R or S configuration, or a mixture of the two. The chiral centers can be further designated as R or S or R,S or d,D, l,L or d,l, D,L.

[0033] In the above formula, the term "C₁ to C₇ alkyl" denotes such radicals as methyl, ethyl, n-propyl, isopropyl, n-butyl, iso-butyl, sec-butyl, tert-butyl, amyl, tert-amyl, hexyl and the like. The preferred "C₁ to C₇ alkyl" groups are methyl, iso-butyl, sec-butyl and iso-propyl.

[0034] The term "C₁ to C₇ substituted alkyl," denotes that the above C₁ to C₇ alkyl groups are substituted by one or more, and preferably one or two, halogen, hydroxy, protected hydroxy, oxo, protected oxo, C₃ to C₇ cycloalkyl, naphthyl, amino, protected amino, (monosubstituted)amino, protected (monosubstituted)amino, (disubstituted)amino, guanidino, protected guanidino, heterocyclic ring, substituted heterocyclic ring, imidazolyl, indolyl, pyrrolidinyl, C₁ to C₇ alkoxy, C₁ to C₇ acyl, C₁ to C₇ acyloxy, nitro, carboxy, protected carboxy, carbamoyl, carboxamide, protected carboxamide, N-(C₁ to C₆ alkyl)carboxamide, protected N-(C₁ to C₆ alkyl)carboxamide, N,N-di(C₁ to C₆ alkyl)carboxamide, cyano, methylsulfonylamino, thiol, C₁ to C₄ alkylthio or C₁ to C₄ alkylsulfonyl groups. The substituted alkyl groups may be substituted once or more, and preferably once or twice, with the same or with different substituents.

[0035] Examples of the above substituted alkyl groups include the 2-oxo-prop-1-yl, 3-oxo-but-1-yl, cyanomethyl, nitromethyl, chloromethyl, hydroxymethyl, tetrahydropyranyloxymethyl, trityloxymethyl, propionyloxymethyl, amino, methylamino, aminomethyl, dimethylamino, carboxymethyl,

allyloxycarbonylmethyl, allyloxycarbonylaminomethyl, methoxymethyl, ethoxymethyl, t-butoxymethyl, acetoxymethyl, chloromethyl, bromomethyl, iodomethyl, trifluoromethyl, 6-hydroxyhexyl, 2,4-dichloro(n-butyl), 2-aminopropyl, 1-chloroethyl, 2-chloroethyl, 1-bromoethyl, 2-chloroethyl, 1-fluoroethyl, 2-fluoroethyl, 1-iodoethyl, 2-iodoethyl, 1-chloropropyl, 2-chloropropyl, 3-chloropropyl, 1-bromopropyl, 2-bromopropyl, 3-bromopropyl, 1-fluoropropyl, 2-fluoropropyl, 3-fluoropropyl, 1-iodopropyl, 2-iodopropyl, 3-iodopropyl, 2-aminoethyl, 1-aminoethyl, N-benzoyl-2-aminoethyl, N-acetyl-2-aminoethyl, N-benzoyl-1-aminoethyl, N-acetyl-1-aminoethyl and the like.

[0036] The term "C₁ to C₇ alkoxy" as used herein denotes groups such as methoxy, ethoxy, n-propoxy, isopropoxy, n-butoxy, t-butoxy and like groups. A preferred alkoxy is methoxy. The term "C₁ to C₇ substituted alkoxy" means the alkyl portion of the alkoxy can be substituted in the same manner as in relation to C₁ to C₇ substituted alkyl. Similarly, the term "C₁ to C₇ phenylalkoxy" as used herein means "C₁ to C₇ alkoxy" bonded to a phenyl radical.

[0037] The substituent term "C₃ to C₇ cycloalkyl" includes the cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl or cycloheptyl rings. The substituent term "C₃ to C₇ substituted cycloalkyl" indicates the above cycloalkyl rings substituted by one or two halogen, hydroxy, protected hydroxy, C₁ to C₄ alkylthio, C₁ to C₄ alkylsulfoxide, C₁ to C₄ alkylsulfonyl, C₁ to C₄ substituted alkylthio, C₁ to C₄ substituted alkylsulfoxide, C₁ to C₄ substituted alkylsulfonyl, C₁ to C₆ alkyl, C₁ to C₇ alkoxy, C₁ to C₆ substituted alkyl, C₁ to C₇ alkoxy, oxo, protected oxo, (monosubstituted)amino, (disubstituted)amino, trifluoromethyl, carboxy, protected carboxy, phenyl, substituted phenyl, phenylthio, phenylsulfoxide, phenylsulfonyl, amino, or protected amino groups.

[0038] The term "substituted phenyl" specifies a phenyl group substituted with one or more, and preferably one or two, moieties chosen from the groups consisting of halogen, hydroxy, protected hydroxy, cyano, nitro, C₁ to C₆ alkyl, C₁ to C₆ substituted alkyl, C₁ to C₇ alkoxy, C₁ to C₇ substituted alkoxy, C₁ to C₇ acyl, C₁ to C₇ substituted acyl, C₁ to C₇ alkylthio, C₁ to C₇ acyloxy, carboxy, protected carboxy, carboxymethyl, protected carboxymethyl, hydroxymethyl, protected

hydroxymethyl, amino, protected amino, (monosubstituted)amino, protected (monosubstituted)amino, (disubstituted)amino, carboxamide, protected carboxamide, N-(C₁ to C₆ alkyl)carboxamide, protected N-(C₁ to C₆ alkyl)carboxamide, N, N-di(C₁ to C₆ alkyl)carboxamide, trifluoromethyl, N-((C₁ to C₆ alkyl)sulfonyl)amino, - (phenylsulfonyl)amino or phenyl, wherein the phenyl is substituted or unsubstituted, such that, for example, a biphenyl results.

[0039] Examples of the term "substituted phenyl" includes a mono- or di(halo)phenyl group such as 2, 3 or 4-chlorophenyl, 2,6-dichlorophenyl, 2,5-dichlorophenyl, 3,4-dichlorophenyl, 2, 3 or 4-bromophenyl, 3,4-dibromophenyl, 3-chloro-4-fluorophenyl, 2, 3 or 4-fluorophenyl and the like; a mono or di(hydroxy)phenyl group such as 2, 3 or 4-hydroxyphenyl, 2,4-dihydroxyphenyl, the protected-hydroxy derivatives thereof and the like; a nitrophenyl group such as 2, 3 or 4-nitrophenyl; a cyanophenyl group, for example, 2, 3 or 4-cyanophenyl; a mono- or di(alkyl)phenyl group such as 2, 3 or 4-methylphenyl, 2,4-dimethylphenyl, 2, 3 or 4-(iso-propyl)phenyl, 2, 3 or 4-ethylphenyl, 2, 3 or 4-(n-propyl)phenyl and the like; a mono or di(alkoxyl)phenyl group, for example, 2,6-dimethoxyphenyl, 2, 3 or 4-methoxyphenyl, 2, 3 or 4-ethoxyphenyl, 2, 3 or 4-(isopropoxy)phenyl, 2, 3 or 4-(t-butoxy)phenyl, 3-ethoxy-4-methoxyphenyl and the like; 2, 3 or 4-trifluoromethylphenyl; a mono- or dicarboxyphenyl or (protected carboxy)phenyl group such as 2, 3 or 4-carboxyphenyl or 2,4-di(protected carboxy)phenyl; a mono-or di(hydroxymethyl)phenyl or (protected hydroxymethyl)phenyl such as 2, 3, or 4-(protected hydroxymethyl)phenyl or 3,4-di(hydroxymethyl)phenyl; a mono- or di(aminomethyl)phenyl or (protected aminomethyl)phenyl such as 2, 3 or 4-(aminomethyl)phenyl or 2,4-(protected aminomethyl)phenyl; or a mono- or di(N-(methylsulfonylamino))phenyl such as 2, 3 or 4-(N-(methylsulfonylamino))phenyl. Also, the term "substituted phenyl" represents disubstituted phenyl groups wherein the substituents are different, for example, 3-methyl-4-hydroxyphenyl, 3-chloro-4-hydroxyphenyl, 2-methoxy-4-bromophenyl, 4-ethyl-2-hydroxyphenyl, 3-hydroxy-4-nitrophenyl, 2-hydroxy 4-chlorophenyl and the like.

[0040] The terms "halo" and "halogen" refer to the fluoro, chloro, bromo or

iodo atoms. There can be one or more halogen, which are the same or different. Preferred halogens are chloro and fluoro.

[0041] The term "substituted amino" refers to an amino group with one substituent chosen from the group consisting of phenyl, substituted phenyl, C₁ to C₆ alkyl, C₁ to C₆ substituted alkyl, C₁ to C₇ acyl, C₁ to C₇ substituted acyl, C₂ to C₇ alkenyl, C₂ to C₇ substituted alkenyl, C₂ to C₇ alkynyl, C₂ to C₇ substituted alkynyl, C₇ to C₁₂ phenylalkyl, C₇ to C₁₂ substituted phenylalkyl and heterocyclic ring. The substituted amino can additionally have an amino-protecting group as encompassed by the term "protected substituted amino."

[0042] The term "(disubstituted)amino" refers to an amino group with two substituents chosen from the group consisting of phenyl, substituted phenyl, C₁ to C₆ alkyl, C₁ to C₆ substituted alkyl, C₁ to C₇ acyl, C₂ to C₇ alkenyl, C₂ to C₇ alkynyl, C₇ to C₁₂ phenylalkyl, and C₇ to C₁₂ substituted phenylalkyl. The two substituents can be the same or different.

[0043] The term "C₁ to C₄ alkylthio" refers to sulfide groups such as methylthio, ethylthio, n-propylthio, isopropylthio, n-butylthio, t-butylthio and like groups.

[0044] The term "C₁ to C₄ substituted alkylthio," denotes that the C₁ to C₄ alkyl portion of this group may be substituted as described above in relation to "substituted alkyl."

[0045] The term "phenoxy" denotes a phenyl bonded to an oxygen atom, wherein the binding to the rest of the molecule is through the oxygen atom. The term "substituted phenoxy" specifies a phenoxy group substituted with one or more, and preferably one or two, moieties chosen from the groups consisting of halogen, hydroxy, protected hydroxy, cyano, nitro, C₁ to C₁₂ alkyl, C₁ to C₁₂ alkoxy, C₁ to C₁₂ substituted alkoxy, C₁ to C₁₂ acyl, C₁ to C₁₂ acyloxy, carboxy, protected carboxy, carboxymethyl, protected carboxymethyl, hydroxymethyl, protected hydroxymethyl, amino, protected amino, (monosubstituted)amino, protected (monosubstituted)amino, (disubstituted)amino, carboxamide, protected carboxamide, N-(C₁ to C₁₂ alkyl)carboxamide, protected N-(C₁ to C₁₂ alkyl)carboxamide, N, N-di(C₁ to C₁₂ alkyl)carboxamide, trifluoromethyl, N-((C₁ to

C₁₂ alkyl)sulfonyl)amino and N- (phenylsulfonyl)amino.

[0046] The terms "C₇ to C₁₈ substituted phenylalkyl" and "C₁ to C₁₂ substituted heterocycloalkyl" denote a C₇ to C₁₈ phenylalkyl group or C₁ to C₁₂ heterocycloalkyl substituted (on the alkyl or, where applicable, phenyl or heterocyclic portion) with one or more, and preferably one or two, groups chosen from halogen, hydroxy, protected hydroxy, oxo, protected oxo, amino, protected amino, substituted amino, protected substituted amino, (disubstituted)amino, guanidino, protected guanidino, heterocyclic ring, substituted heterocyclic ring, C₁ to C₁₂ alkyl, C₁ to C₁₂ substituted alkyl, C₁ to C₁₂ alkoxy, C₁ to C₁₂ substituted alkoxy, C₁ to C₁₂ acyl, C₁ to C₁₂ substituted acyl, C₁ to C₁₂ acyloxy, nitro, carboxy, protected carboxy, carbamoyl, carboxamide, protected carboxamide, N-(C₁ to C₁₂ alkyl)carboxamide, protected N-(C₁ to C₁₂ alkyl)carboxamide, N, N-(C₁ to C₁₂ dialkyl)carboxamide, cyano, N-(C₁ to C₁₂ alkylsulfonyl)amino, thiol, C₁ to C₁₀ alkylthio, C₁ to C₁₀ alkylsulfonyl groups; and/or the phenyl group may be substituted with one or more, and preferably one or two, substituents chosen from halogen, hydroxy, protected hydroxy, cyano, nitro, C₁ to C₁₂ alkyl, C₁ to C₁₂ substituted alkyl, C₁ to C₁₂ alkoxy, C₁ to C₁₂ substituted alkoxy, C₁ to C₁₂ acyl, C₁ to C₁₂ substituted acyl, C₁ to C₁₂ acyloxy, carboxy, protected carboxy, carboxymethyl, protected carboxymethyl, hydroxymethyl, protected hydroxymethyl, amino, protected amino, (monosubstituted)amino, protected (monosubstituted)amino, (disubstituted)amino, carboxamide, protected carboxamide, N-(C₁ to C₁₂ alkyl)carboxamide, protected N-(C₁ to C₁₂ alkyl)carboxamide, N, N-di(C₁ to C₁₂ alkyl)carboxamide, trifluoromethyl, N-((C₁ to C₁₂ alkyl)sulfonyl)amino, N-(phenylsulfonyl)amino, cyclic C₂ to C₁₂ alkylene or a phenyl group, substituted or unsubstituted, for a resulting biphenyl group. The substituted alkyl, phenyl or heterocyclic groups may be substituted with one or more, and preferably one or two, substituents which can be the same or different.

[0047] Examples of the term "C₇ to C₁₈ substituted phenylalkyl" include groups such as 2-phenyl-1-chloroethyl, 2-(4-methoxyphenyl)ethyl, 4-(2,6-dihydroxy phenyl)n-hexyl, 2-(5-cyano-3-methoxyphenyl)n-pentyl, 3-(2,6-dimethylphenyl)n-propyl, 4-chloro-3-aminobenzyl, 6-(4-methoxyphenyl)-3-carboxy(n-hexyl), 5-(4-

aminomethylphenyl)- 3-(aminomethyl)n-pentyl, 5-phenyl-3-oxo-n-pent-1-yl and the like.

[0048] The term "C₇ to C₁₈ phenylalkylene" specifies a C₇ to C₁₈ phenylalkyl, as defined above, where the phenylalkyl radical is bonded at two different positions connecting together two separate additional groups. The definition includes groups of the formula: -phenyl-alkyl-, -alkyl-phenyl- and -alkyl-phenyl-alkyl-. Substitutions on the phenyl ring can be 1,2, 1,3 or 1,4.

[0049] C₇ to C₁₈ phenylalkylenes include, for example, 1,4-tolylene and 1,3-xylylene.

[0050] The terms "cyclic C₂ to C₇ alkylene," "substituted cyclic C₂ to C₇ alkylene," "cyclic C₂ to C₇ heteroalkylene," and "substituted cyclic C₂ to C₇ heteroalkylene," defines such a cyclic group bonded ("fused") to the phenyl radical resulting in a bicyclic ring system. The cyclic group may be saturated or contain one or two double bonds. Furthermore, the cyclic group may have one or two methylene or methine groups replaced by one or two oxygen, nitrogen or sulfur atoms which are the cyclic C₂ to C₇ heteroalkylene.

[0051] The cyclic alkylene or heteroalkylene group may be substituted once or twice by the same or different substituents which, if appropriate, can be connected to another part of the compound (e.g., alkylene) selected from the group consisting of the following moieties: hydroxy, protected hydroxy, carboxy, protected carboxy, oxo, protected oxo, C₁ to C₄ acyloxy, formyl, C₁ to C₁₂ acyl, C₁ to C₁₂ alkyl, C₁ to C₇ alkoxy, C₁ to C₁₀ alkylthio, C₁ to C₁₀ alkylsulfoxide, C₁ to C₁₀ alkylsulfonyl, halo, amino, protected amino, substituted amino, protected substituted amino, (disubstituted)amino, hydroxymethyl or a protected hydroxymethyl.

[0052] The cyclic alkylene or heteroalkylene group fused onto the benzene radical can contain two to ten ring members, but it preferably contains three to six members. Examples of such saturated cyclic groups are when the resultant bicyclic ring system is 2,3-dihydro-indanyl and a tetralin ring. When the cyclic groups are unsaturated, examples occur when the resultant bicyclic ring system is a naphthyl ring or indolyl. Examples of fused cyclic groups which each contain

one nitrogen atom and one or more double bond, preferably one or two double bonds, are when the benzene radical is fused to a pyridino, pyrano, pyrrolo, pyridinyl, dihydropyrrolo, or dihydropyridinyl ring. Examples of fused cyclic groups which each contain one oxygen atom and one or two double bonds are when the benzene radical ring is fused to a furo, pyrano, dihydrofurano, or dihydropyrano ring. Examples of fused cyclic groups which each have one sulfur atom and contain one or two double bonds are when the benzene radical is fused to a thieno, thiopyrano, dihydrothieno or dihydrothiopyrano ring. Examples of cyclic groups which contain two heteroatoms selected from sulfur and nitrogen and one or two double bonds are when the benzene radical ring is fused to a thiazolo, isothiazolo, dihydrothiazolo or dihydroisothiazolo ring. Examples of cyclic groups which contain two heteroatoms selected from oxygen and nitrogen and one or two double bonds are when the benzene ring is fused to an oxazolo, isoxazolo, dihydrooxazolo or dihydroisoxazolo ring. Examples of cyclic groups which contain two nitrogen heteroatoms and one or two double bonds occur when the benzene ring is fused to a pyrazolo, imidazolo, dihydropyrazolo or dihydroimidazolo ring or pyrazinyl.

[0053] The term "heterocycle" or "heterocyclic ring" denotes optionally substituted five-membered to eight-membered rings that have 1 to 4 heteroatoms, such as oxygen, sulfur and/or nitrogen, in particular nitrogen, either alone or in conjunction with sulfur or oxygen ring atoms. These five-membered to eight-membered rings may be saturated, fully unsaturated or partially unsaturated, with fully saturated rings being preferred. Preferred heterocyclic rings include morpholino, piperidinyl, piperazinyl, 2-amino-imidazolyl, tetrahydrofurano, pyrrolo, tetrahydrothiophen-yl, hexylmethyleneimino and heptylmethyleneimino.

[0054] The term "substituted heterocycle" or "substituted heterocyclic ring" means the above-described heterocyclic ring is substituted with, for example, one or more, and preferably one or two, substituents which are the same or different which substituents can be halogen, hydroxy, protected hydroxy, cyano, nitro, C₁ to C₁₂ alkyl, C₁ to C₁₂ alkoxy, C₁ to C₁₂ substituted alkoxy, C₁ to C₁₂ acyl,

C₁ to C₁₂ acyloxy, carboxy, protected carboxy, carboxymethyl, protected carboxymethyl, hydroxymethyl, protected hydroxymethyl, amino, protected amino, substituted amino, protected substituted amino, (disubstituted)amino carboxamide, protected carboxamide, N-(C₁ to C₁₂ alkyl)carboxamide, protected N-(C₁ to C₁₂ alkyl)carboxamide, N, N-di(C₁ to C₁₂ alkyl)carboxamide, trifluoromethyl, N-((C₁ to C₁₂ alkyl)sulfonyl)amino, N-(phenylsulfonyl)amino, heterocycle or substituted heterocycle groups.

[0055] One or more of the compounds of the invention, even within a given library, may be present as a salt. The term "salt" encompasses those salts that form with the carboxylate anions and amine nitrogens and include salts formed with the organic and inorganic anions and cations discussed below. Furthermore, the term includes salts that form by standard acid-base reactions with basic groups (such as amino groups) and organic or inorganic acids. Such acids include hydrochloric, sulfuric, phosphoric, acetic, succinic, citric, lactic, maleic, fumaric, palmitic, cholic, pamoic, mucic, D-glutamic, D-camphoric, glutaric, phthalic, tartaric, lauric, stearic, salicylic, methanesulfonic, benzenesulfonic, sorbic, picric, benzoic, cinnamic, and like acids.

[0056] The term "organic or inorganic cation" refers to counter-ions for the carboxylate anion of a carboxylate salt. The counter-ions are chosen from the alkali and alkaline earth metals, (such as lithium, sodium, potassium, barium, aluminum and calcium); ammonium and mono-, di- and tri-alkyl amines such as trimethylamine, cyclohexylamine; and the organic cations, such as dibenzylammonium, benzylammonium, 2-hydroxyethylammonium, bis(2-hydroxyethyl)ammonium, phenylethylbenzylammonium, dibenzylethylenediammonium, and like cations. See, for example, "Pharmaceutical Salts," Berge et al., J. Pharm. Sci., 66:1-19 (1977). Other cations encompassed by the above term include the protonated form of procaine, quinine and N-methylglucosamine, and the protonated forms of basic amino acids such as glycine, ornithine, histidine, phenylglycine, lysine and arginine. Furthermore, any zwitterionic form of the instant compounds formed by a carboxylic acid and an amino group is referred to by this term. For example, a

cation for a carboxylate anion will exist when R_2 or R_3 is substituted with a (quaternary ammonium)methyl group. A preferred cation for the carboxylate anion is the sodium cation.

[0057] The compounds of the invention can also exist as solvates and hydrates. Thus, these compounds may crystallize with, for example, waters of hydration, or one, a number of, or any fraction thereof of molecules of the mother liquor solvent. The solvates and hydrates of such compounds are included within the scope of this invention.

[0058] One or more compounds of the invention, even when in a library, can be in the biologically active ester form, such as the non-toxic, metabolically-labile ester-form. Such ester forms induce increased blood levels and prolong the efficacy of the corresponding non-esterified forms of the compounds. Ester groups which can be used include the lower alkoxymethyl groups, for example, methoxymethyl, ethoxymethyl, isopropoxymethyl and the like; the $-(C_1 \text{ to } C_7)$ alkoxyethyl groups, for example methoxyethyl, ethoxyethyl, propoxyethyl, isopropoxyethyl and the like; the 2-oxo-1,3-dioxolen-4-ylmethyl groups, such as 5-methyl-2-oxo-1,3-dioxolen-4-ylmethyl, 5-phenyl-2-oxo-1,3-dioxolen-4-ylmethyl and the like; the C_1 to C_4 alkylthiomethyl groups, for example methylthiomethyl, ethylthiomethyl, iso-propylthiomethyl and the like; the acyloxymethyl groups, for example pivaloyloxymethyl, pivaloyloxyethyl, -acetoxymethyl and the like; the ethoxycarbonyl-1-methyl group; the -acetoxylethyl; the 1- $(C_1 \text{ to } C_7 \text{ alkyloxycarbonyloxy})$ ethyl groups such as the 1-(ethoxycarbonyloxy)ethyl group; and the 1- $(C_1 \text{ to } C_7 \text{ alkylaminocarbonyloxy})$ ethyl groups such as the 1-(methylaminocarbonyloxy)ethyl group.

[0059] The term "amino acid" includes any one of the twenty naturally-occurring amino acids or the D-form of any one of the naturally-occurring amino acids. In addition, the term "amino acid" also includes other non-naturally occurring amino acids besides the D-amino acids, which are functional equivalents of the naturally-occurring amino acids. Such non-naturally-occurring amino acids include, for example, norleucine ("Nle"), norvaline ("Nva"), L- or D-naphthalanine, ornithine ("Orn"), homoarginine (homoArg) and others well known

in the peptide art, such as those described in M. Bodanzsky, "Principles of Peptide Synthesis," 1st and 2nd revised ed., Springer-Verlag, New York, NY, 1984 and 1993, and Stewart and Young, "Solid Phase Peptide Synthesis," 2nd ed., Pierce Chemical Co., Rockford, IL, 1984. Amino acids and amino acid analogs can be purchased commercially (Sigma Chemical Co.; Advanced Chemtech) or synthesized using methods known in the art.

[0060] The term "functionalized resin" means any resin, crosslinked or otherwise, where functional groups have been introduced into the resin, as is common in the art. Such resins include, for example, those functionalized with amino, alkylhalo, formyl or hydroxy groups. Such resins which can serve as solid supports are well known in the art and include, for example, 4-methylbenzhydrylamine-copoly(styrene-1% divinylbenzene) (MBHA), 4-hydroxymethylphenoxymethyl-copoly(styrene-1% divinylbenzene), 4-oxymethyl-phenyl-acetamido-copoly(styrene-1% divinylbenzene)(Wang), 4-(oxymethyl)-phenylacetamido methyl (Pam), and TentagelTM, from Rapp Polymere GmbH, trialkoxy-diphenyl-methyl ester- copoly(styrene-1% divinylbenzene)(RINK) all of which are commercially available. Other functionalized resins are known in the art and can be use without departure from the scope of the current invention. Such resins may include those described in Jung, G., Combinatorial Peptide and Nonpeptide Libraries, A Handbook (VCH Verlag, 1996) or Bunin, B. A., The Combinatorial Index (Academic Press, 1998).

[0061] As used herein, a "combinatorial library" is an intentionally created collection of differing molecules which can be prepared by the means provided below or otherwise and screened for biological activity in a variety of formats (e.g., libraries of soluble molecules, libraries of compounds attached to resin beads, silica chips or other solid supports). A "combinatorial library," as defined above, involves successive rounds of chemical syntheses based on a common starting structure. The combinatorial libraries can be screened in any variety of assays, such as those detailed below as well as others useful for assessing their biological activity. The combinatorial libraries will generally have at least one active compound and are generally prepared such that the compounds are in

[0068] Powders and tablets preferably contain between about 5% to about 70% by weight of the active ingredient. Suitable carriers include, for example, magnesium carbonate, magnesium stearate, talc, lactose, sugar, pectin, dextrin, starch, tragacanth, methyl cellulose, sodium carboxymethyl cellulose, a low-melting wax, cocoa butter and the like.

[0069] The pharmaceutical compositions can include the formulation of the active compound with encapsulating material as a carrier providing a capsule in which the active component (with or without other carriers) is surrounded by a carrier, which is thus in association with it. In a similar manner, cachets are also included. Tablets, powders, cachets, and capsules can be used as solid dosage forms suitable for oral administration.

[0070] Liquid pharmaceutical compositions include, for example, solutions suitable for oral or parenteral administration, or suspensions, and emulsions suitable for oral administration. Sterile water solutions of the active component or sterile solutions of the active component in solvents comprising water, ethanol, or propylene glycol are examples of liquid compositions suitable for parenteral administration.

[0071] Sterile solutions can be prepared by dissolving the active component in the desired solvent system, and then passing the resulting solution through a membrane filter to sterilize it or, alternatively, by dissolving the sterile compound in a previously sterilized solvent under sterile conditions.

[0072] Aqueous solutions for oral administration can be prepared by dissolving the active compound in water and adding suitable flavorants, coloring agents, stabilizers, and thickening agents as desired. Aqueous suspensions for oral use can be made by dispersing the finely divided active component in water together with a viscous material such as natural or synthetic gums, resins, methyl cellulose, sodium carboxymethyl cellulose, and other suspending agents known to the pharmaceutical formulation art.

[0073] Preferably, the pharmaceutical composition is in unit dosage form. In such form, the composition is divided into unit doses containing appropriate quantities of the active piperidine-3-carboxamide. The unit dosage form can be a

packaged preparation, the package containing discrete quantities of the preparation, for example, packeted tablets, capsules, and powders in vials or ampules. The unit dosage form can also be a capsule, cachet, or tablet itself, or it can be the appropriate number of any of these packaged forms.

[0074] As pharmaceutical compositions for treating infections, pain, or any other indication the compounds of the present invention are generally in a pharmaceutical composition so as to be administered to a subject at dosage levels of from 0.7 to 7000 mg per day, and preferably 1 to 500 mg per day, for a normal human adult of approximately 70 kg of body weight, this translates into a dosage of from 0.01 to 100 mg/kg of body weight per day. The specific dosages employed, however, can be varied depending upon the requirements of the patient, the severity of the condition being treated, and the activity of the compound being employed. The determination of optimum dosages for a particular situation is within the skill of the art.

[0075] Variant piperidine-3-carboxamide derivative compounds and combinatorial libraries can be prepared as shown in figures 1 and 2 in order to achieve a high level of diversity.

[0076] Resins suitable for use in the present invention can easily be determined by one skilled in the art. Such resins include but are not limited to polystyrene resin (e.g. Wang resin : *p*-benzyloxybenzyl alcohol-polystyrene) and PEG-grafted polystyrene resin (e.g. Tentagel, Argogel).

[0077] Other suitable resins known in the art can be found in "Solid Phase Synthesis and Combinatorial Technologies", Seneci, P.; John Wiley and Sons, 2000, p 1-45.

[0078] The resulting compound can be cleaved from the resin. Resin-bound piperidine-3-carboxamide derivative compounds can be cleaved by treating them, for example, with HF. They can also be cleaved with TFA/DCM, provided that TFA sensitive protecting group such as Boc are not used in the synthetic scheme. The compounds can be extracted from the spent resin, for example, with AcOH.

[0079] The nonsupport-bound combinatorial libraries can be screened as

single compounds. In addition, the nonsupport-bound combinatorial libraries can be screened as mixtures in solution in assays such as radio-receptor inhibition assays, anti-bacterial assays, anti-fungal assays, calmodulin-dependent phosphodiesterase (CaMPDE) assays and phosphodiesterase (PDE) assays, as described in detail below. Deconvolution of highly active mixtures can then be carried out by iterative or positional scanning methods. These techniques, the iterative approach or the positional scanning approach, can be utilized for finding other active compounds within the combinatorial libraries of the present invention using any one of the below-described assays or others well known in the art.

[0080] The iterative approach is well-known and is set forth in general in Houghten *et al.*, *Nature*, 354, 84-86 (1991) and Dooley *et al.*, *Science*, 266, 2019-2022 (1994), both of which are incorporated herein by reference. In the iterative approach, for example, sub-libraries of a molecule having three variable groups are made wherein the first variable is defined. Each of the compounds with the defined variable group is reacted with all of the other possibilities at the other two variable groups. These sub-libraries are each tested to define the identity of the second variable in the sub-library having the highest activity in the screen of choice. A new sub-library with the first two variable positions defined is reacted again with all the other possibilities at the remaining undefined variable position. As before, the identity of the third variable position in the sub-library having the highest activity is determined. If more variables exist, this process is repeated for all variables, yielding the compound with each variable contributing to the highest desired activity in the screening process. Promising compounds from this process can then be synthesized on larger scale in traditional single-compound synthetic methods for further biological investigation.

[0081] The positional-scanning approach has been described for various combinatorial libraries as described, for example, in R. Houghten *et al.* PCT/US91/08694 and U.S. Patent 5,556,762, both of which are incorporated herein by reference. In the positional scanning approach, sublibraries are made defining only one variable with each set of sublibraries and all possible sublibraries with each single variable defined (and all other possibilities at all of

the other variable positions), made and tested. From the instant description one skilled in the art could synthesize combinatorial libraries wherein two fixed positions are defined at a time. From the testing of each single-variable defined combinatorial library, the optimum substituent at that position can be determined, pointing to the optimum or at least a series of compounds having a maximum of the desired biological activity. Thus, the number of sublibraries for compounds with a single position defined will be the number of different substituents desired at that position, and the number of all the compounds in each sublibrary will be the product of the number of substituents at each of the other variables.

[0082] Individual compounds and pharmaceutical compositions containing the compounds, as well as methods of using the same, are included within the scope of the present invention. The compounds of the present invention can be used for a variety of purposes and indications and as medicaments for any such purposes and indications. For example, piperidine-3-carboxamide derivative compounds of the present invention can be used as pesticides, acaricides, receptor agonists or antagonists and antimicrobial agents, including antibacterial or antiviral agents. The libraries can be screened in any variety of melanocortin receptor and related activity assays, such as those detailed below as well as others known in the art. Additionally, the subject compounds can be useful as analgesics. Assays which can be used to test the biological activity of the instant compounds include antimicrobial assays, a competitive enzyme-linked immunoabsorbent assay and radio-receptor assays, as described below.

[0083] The melanocortin (MC) receptors are a group of cell surface proteins that mediate a variety of physiological effects, including regulation of adrenal gland function such as production of the glucocorticoids cortisol and aldosterone; control of melanocyte growth and pigment production; thermoregulation; immunomodulation; and analgesia. Five distinct MC receptors have been cloned and are expressed in a variety of tissues, including melanocytes, adrenal cortex, brain, gut, placenta, skeletal muscle, lung, spleen, thymus, bone marrow, pituitary, gonads and adipose tissue (Tatro, Neuroimmunomodulation 3:259-284 (1996)). Three MC receptors, MCR-1, MCR-3 and MCR-4, are expressed in

brain tissue (Xia et al., Neuroreport 6:2193-2196 (1995)).

[0084] A variety of ligands termed melanocortins function as agonists that stimulate the activity of MC receptors. The melanocortins include melanocyte-stimulating hormones (MSH) such as α -MSH, β -MSH and γ -MSH, as well as adrenocorticotrophic hormone (ACTH). Individual ligands can bind to multiple MC receptors with differing relative affinities. The variety of ligands and MC receptors with differential tissue-specific expression likely provides the molecular basis for the diverse physiological effects of melanocortins and MC receptors. For example, α -MSH antagonizes the actions of immunological substances such as cytokines and acts to modulate fever, inflammation and immune responses (Catania and Lipton, Annals N. Y. Acad. Sci. 680:412-423 (1993)).

[0085] The role of certain specific MC receptors in some of the physiological effects described above for MC receptors has been elucidated. For example, MCR-1 is involved in pain and inflammation. MCR-1 mRNA is expressed in neutrophils (Catania et al., Peptides 17:675-679 (1996)). The anti-inflammatory agent α -MSH was found to inhibit migration of neutrophils. Thus, the presence of MCR-1 in neutrophils correlates with the anti-inflammatory activity of α -MSH.

[0086] An interesting link of MC receptors to regulation of food intake and obesity has recently been described. The brain MC receptor MCR-4 has been shown to function in the regulation of body weight and food intake. Mice in which MCR-4 has been knocked out exhibit weight gain (Huszar et al., Cell 88:131-141 (1997)). In addition, injection into brain of synthetic peptides that mimic melanocortins and bind to MCR-4 caused suppressed feeding in normal and mutant obese mice (Fan et al., Nature 385:165-168 (1997)). These results indicate that the brain MC receptor MCR-4 functions in regulating food intake and body weight.

[0087] Due to the varied physiological activities of MC receptors, high affinity ligands of MC receptors could be used to exploit the varied physiological responses of MC receptors by functioning as potential therapeutic agents or as lead compounds for the development of therapeutic agents. Furthermore, due to

MCR-4 ligands are useful for treating obesity. The binding characteristics and specificity of a given MC receptor ligand can be selected based on the particular disease or physiological effect that is desired to be altered.

[0091] Another assay useful for identifying or characterizing MC receptor ligands measures signaling of MC receptors. MC receptors are G protein-coupled receptors that couple to adenylate cyclase and produce cAMP. Therefore, measuring cAMP production in a cell expressing a MC receptor and treated with a MC receptor ligand can be used to assess the function of the MC receptor ligand in activating a MC receptor.

[0092] Ligands for MC-3 that can alter the activity of an MC-3 receptor can be useful for treating sexual dysfunction and other conditions or conditions associated with MC-3 such as inflammation. Other MC-3-associated conditions that can be treated with the MC-3 receptor ligands include disuse deconditioning; organ damage such as organ transplantation or ischemic injury; adverse reactions associated with cancer chemotherapy; diseases such as atherosclerosis that are mediated by free radicals and nitric oxide action; bacterial endotoxic sepsis and related shock; adult respiratory distress syndrome; and autoimmune or other patho-immunogenic diseases or reactions such as allergic reactions or anaphylaxis, rheumatoid arthritis, inflammatory bowel disease, ulcerative colitis, glomerulonephritis, systemic lupus erythematosus, transplant atherosclerosis and parasitic mediated immune dysfunctions such as Chagas's disease.

[0093] The invention further provides a method for treating an MC-3-associated condition in a subject. The term "MC-3-associated condition" includes any condition or condition mediated by MC-3 or can be affected by binding an MC-3 ligand. Such conditions include inflammation and sexual dysfunction.

[0094] The term "sexual dysfunction" herein means any condition that inhibits or impairs normal sexual function, including coitus. However, the term need not be limited to physiological conditions, but may include psychogenic conditions or perceived impairment without a formal diagnosis of pathology.

[0095] In males, sexual dysfunction includes erectile dysfunction. The term "erectile dysfunction" or "impotence" means herein the inability or impaired ability to attain or sustain an erection that would be of satisfactory rigidity for coitus. Sexual dysfunction in males can also include premature ejaculation and priapism, which is a condition of prolonged and sometimes painful erection unrelated to sexual activity, often associated with sickle-cell disease.

[0096] In females, sexual dysfunction includes sexual arousal disorder. The term "sexual arousal disorder" means herein a persistent or recurrent failure to attain or maintain the lubrication-swelling response of sexual excitement until completion of sexual activity. Sexual dysfunction in females can also include inhibited orgasm and dyspareunia, which is painful or difficult coitus. Sexual dysfunction can also be manifested as inhibited sexual desire or inhibited lordosis behavior in animals.

[0097] In addition, the ability of the compounds to inhibit bacterial growth, and therefore be useful to that infection, can be determined by methods well known in the art. Compounds of the present invention can be shown to have antimicrobial activity by the *in vitro* antimicrobial activity assay described below and, therefore, are useful as antimicrobial agents.

[0098] Moreover, an exemplary *in vitro* antimicrobial activity assay is described in Blondelle and Houghten, *Biochemistry* 30:4671-4678 (1991), which is incorporated herein by reference. In brief, *Staphylococcus aureus* ATCC 29213 (Rockville, MD) is grown overnight at 37°C in Mueller-Hinton broth, then re-inoculated and incubated at 37°C to reach the exponential phase of bacterial growth (i.e., a final bacterial suspension containing 10⁵ to 5 x 10⁵ colony-forming units/ml). The concentration of cells is established by plating 100 µl of the culture solution using serial dilutions (e.g., 10⁻², 10⁻³ and 10⁻⁴) onto solid agar plates. In 96-well tissue culture plates, compounds, individual or in mixtures, are added to the bacterial suspension at concentrations derived from serial two-fold dilutions ranging from 1500 to 2.9 µg/ml. The plates are incubated overnight at 37°C and the growth determined at each concentration by OD₆₂₀ nm. The IC₅₀

(the concentration necessary to inhibit 50% of the growth of the bacteria) can then be calculated.

[0099] The competitive ELISA method which can be used here is a modification of the direct ELISA technique described previously in Appel et al., J. Immunol. 144:976-983 (1990), which is incorporated herein by reference. It differs only in the MAb addition step. Briefly, multi-well microplates are coated with the antigenic peptide (Ac-GASPYPNLSNQQT-NH₂) at a concentration of 100 pmol/50 μ l. After blocking, 25 μ l of a 1.0 mg/ml solution of each mixture of a synthetic combinatorial library (or individual compound) is added, followed by MAb 125-10F3 (Appel et al., *supra*) (25 μ l per well). The MAb is added at a fixed dilution in which the bicyclic guanidine in solution effectively competes for MAb binding with the antigenic peptide adsorbed to the plate. The remaining steps are the same as for direct ELISA. The concentration of compound necessary to inhibit 50% of the MAb binding to the control peptide on the plate (IC₅₀) is determined by serial dilutions of the compound.

[0100] Alternative screening can be done with radio-receptor assays. The radio-receptor assay, can be selective for any one of the μ , κ , or δ opiate receptors. Compounds of the present invention can be useful *in vitro* for the diagnosis of relevant opioid receptor subtypes, such as κ , in the brain and other tissue samples. Similarly, the compounds can be used *in vivo* diagnostically to localize opioid receptor subtypes.

[0101] The radio-receptor assays are also an indication of the compounds' analgesic properties as described, for example, in Dooley et al., *Proc. Natl. Acad. Sci.*, 90:10811-10815 (1993). For example, it can be envisioned that these compounds can be used for therapeutic purposes to block the peripheral effects of a centrally acting pain killer. For instance, morphine is a centrally acting pain killer. Morphine, however, has a number of deleterious effects in the periphery which are not required for the desired analgesic effects, such as constipation and pruritus (itching). While it is known that the many compounds do not readily cross the blood-brain barrier and, therefore, elicit no central effect, the subject

compounds can have value in blocking the periphery effects of morphine, such as constipation and pruritus. Accordingly, the subject compounds can also be useful as drugs, namely as analgesics, or to treat pathologies associated with other compounds which interact with the opioid receptor system.

[0102] Additionally, such compounds can be tested in a σ receptor assay. Ligands for the σ receptor can be useful as antipsychotic agents, as described in Abou-Gharbia et al., *Annual Reports in Medicinal Chemistry*, 28:1-10 (1993).

[0103] Radio-receptor assays can be performed with particulate membranes prepared using a modification of the method described in Pasternak et al., *Mol. Pharmacol.* 11:340-351 (1975), which is incorporated herein by reference. Rat brains frozen in liquid nitrogen can be obtained from Rockland (Gilbertsville, PA). The brains are thawed, the cerebella removed and the remaining tissue weighed. Each brain is individually homogenized in 40 ml Tris-HCl buffer (50 mM, pH 7.4, 4°C) and centrifuged (Sorvall® RC5C SA-600: Du Pont, Wilmington, DE) (16,000 rpm) for 10 minutes. The pellets are resuspended in fresh Tris-HCl buffer and incubated at 37°C for 40 minutes. Following incubation, the suspensions are centrifuged as before, the resulting pellets resuspended in 100 volumes of Tris buffer and the suspensions combined. Membrane suspensions are prepared and used in the same day. Protein content of the crude homogenates generally range from 0.15-0.2 mg/ml as determined using the method described in Bradford, M.M., *Anal. Biochem.* 72:248-254 (1976), which is incorporated herein by reference.

[0104] Binding assays are carried out in polypropylene tubes, each tube containing 0.5 ml of membrane suspension. 8 nM of 3H-[D-Ala²,Me-Phe⁴,Gly⁵]enkephalin (DAMGO) (specific activity = 36 Ci/mmol, 160,000 cpm per tube; which can be obtained from Multiple Peptide Systems, San Diego, CA, through NIDA drug distribution program 271-90-7302) and 80 µg/ml of bicyclic guanidine, individual or as a mixture and Tris-HCl buffer in a total volume of 0.65 ml. Assay tubes are incubated for 60 mins. at 25°C. The reaction is terminated by filtration through GF-B filters on a Tomtec harvester (Orange, CT). The filters are

subsequently washed with 6 ml of Tris-HCl buffer, 4°C. Bound radioactivity is counted on a Pharmacia Biotech Betaplate Liquid Scintillation Counter (Piscataway, NJ) and expressed in cpm. To determine inter- and intra-assay variation, standard curves in which 3H-DAMGO is incubated in the presence of a range of concentrations of unlabeled DAMGO (0.13-3900 nM) are generally included in each plate of each assay (a 96-well format). Competitive inhibition assays are performed as above using serial dilutions of the piperidine-3-carboxamides, individually or in mixtures. IC₅₀ values (the concentration necessary to inhibit 50% of 3H-DAMGO binding) are then calculated. IC₅₀ values of less than 1000 nM are indicative of highly active opioid compounds which bind to the μ receptor, with particularly active compounds having IC₅₀ values of 100 nM or less and the most active compounds with values of less than 10 nM.

[0105] As opposed to this μ receptor selective assay, which can be carried out using 3H-DAMGO as radioligand, as described above, assays selective for κ receptors can be carried out using [3H]-U69,593 (3 nM, specific activity 62 Ci/mmol) as radioligand. Assays selective for δ opiate receptors can be carried out using tritiated DSLET ([D-Ser2, D-Leu5]-threonine-enkephalin) as radioligand. Assays selective for the σ opiate receptor can use radiolabeled pentazocine as ligand.

[0106] Screening of combinatorial libraries and compounds of the invention can be done with an anti-fungal assay. Compounds of the present invention can be useful for treating fungal infections.

[0107] Screening of combinatorial libraries and compounds of the invention also can be done with a calmodulin-dependent phosphodiesterase (CaMPDE) assay. Compounds of the present invention can be useful as calmodulin antagonists.

[0108] Calmodulin (CaM), which is the major intracellular calcium receptor, is involved in many processes that are crucial to cellular viability. In particular, calmodulin is implicated in calcium-stimulated cell proliferation. Calmodulin

antagonists are, therefore, useful for treating conditions associated with increased cell proliferation, for example, cancer. In addition, calmodulin antagonists such as compounds of the subject invention are useful both in vitro and in vivo for identifying the role of calmodulin in other biological processes. The disadvantages of known antagonists such as trifluoperazine and N-(4-aminobutyl)-5-chloro-2-naphthalenesulfonamide (W13) include their non-specificity and toxicity. In contrast, advantages of the combinatorial libraries and compounds of the subject invention as calmodulin antagonists include their reduced flexibility and ability to generate broader conformational space of interactive residues as compared to their linear counterparts.

[0109] An example of an assay that identifies CaM antagonists is a CaMPDE assay. In brief, samples are mixed with 50 μ l of assay buffer (360 mM Tris, 360 mM Imidazole, 45 mM $\text{Mg}(\text{CH}_3\text{COO})_2$, pH 7.5) and 10 μ l of CaCl_2 (4.5 mM) to a final volume of 251 μ l. 25 μ l of calmodulin stock solution (Boehringer Mannheim; 0.01 $\mu\text{g}/\mu\text{l}$) is then added and the samples then sit at room temperature for 10 minutes. 14 μ l of PDE (Sigma; 2 Units dissolved in 4 ml of water; stock concentration: 0.0005 Units/ μ l) is then added, followed by 50 μ l of 5'-nucleotidase (Sigma; 100 Units dissolved in 10 ml of 10 mM Tris-HCl containing 0.5 mM $\text{Mg}(\text{CH}_3\text{COO})_2$, pH 7.0; stock concentration: 10 Units/ml). The samples are then incubated for 10 minutes at 30°C. 50 μ l of adenosine 3',5'-cyclic monophosphate (cAMP) (20 mM in water at pH 7.0) is added, the samples incubated for 1 hour at 30°C and then vortexed. 200 μ l of trichloroacetic acid (TCA) (55% in water) is added to a 200 μ l sample aliquot, which is then vortexed and centrifuged for 10 minutes. 80 μ l of the resulting supernatants of each sample is transferred to a 96-well plate, with 2 wells each containing 80 μ l of each sample. 80 μ l of ammonium molybdate (1.1% in 1.1N H_2SO_4) is then added to all the wells, and the OD of each were determined at 730nm, with the values later subtracted to the final OD reading. 16 μ l of reducing agent (6g sodium bisulfite, 0.6g sodium sulfite and 125mg of 1-amino-2-naphtol-4-sulfonic acid in 50ml of water) is then added to one of each sample duplicate and 16 μ l of water is added to the other duplicate. After sitting for 1 hour at room

temperature, the OD of each well is determined at 730nm. The percent inhibition of calmodulin activity is then calculated for each sample, using as 0% inhibition a control sample containing all reagents without any test samples and as 100% inhibition a control sample containing test samples and all reagents except calmodulin. In addition, the percent inhibition of phosphodiesterase activity was determined by following a similar protocol as the CaMPDE assay described above, except not adding calmodulin to the sample mixture and calculating the percent inhibition by using as 0% inhibition a control reagent without any test samples and as 100% inhibition a control sample containing test samples and all reagents except cAMP.

[0110] The following examples are provided to illustrate but not limit the present invention. The following abbreviations have the corresponding meanings:

DMF : N,N-dimethylformamide;

HOBt : 1-hydroxybenzotriazole;

Boc : tert-butoxycarbonyl;

DIC : N,N--diisopropylcarbodiimide;

TFA : trifluoroacetic acid;

DIEA : N,N-diisopropylethylamine;

DCM : dichloromethane;

RT : room temperature

MeOH: methanol

MeOEtOH : 2-methoxyethanol

DCE : 1,2-dichloroethane

THF : tetrahydrofuran

ACN : acetonitrile

Wang resin : *p*-benzyloxybenzyl alcohol-polystyrene Br-Wang resin :

p-benzyloxybenzyl bromide-polystyrene

PP : polypropylene

PPh₃Br₂ : triphenylphosphine dibromide

DMAP : 4-dimethylamino-pyridine

Example 1

Synthetic Protocol

Step 1a. Loading Hydroxybenzaldehydes on Bromo-Wang Resin

[0111] A 1 L Pyrex media bottle was charged with 100 g Bromo-Wang resin (100-200 mesh, 1.4 mmol/g). DMF (350 ml) was added and the bottle was shaken by hand to distribute the solvent within the swollen resin. A 500 ml Pyrex media bottle was charged with the hydroxybenzaldehyde (420 mmol, 3 eq) and the aldehyde was dissolved in DMF (300 ml). The aldehyde solution was cooled to 0° C (ice bath) and potassium *tert*-butoxide (44.8 g, 400 mmol) was added in two equal portions shaking for about 5 min. between additions. CAUTION: EXOTHERMIC REACTION. The temperature must be maintained at or below 25° C. The bottle was removed from the ice bath and shaken periodically to help dissolve the potassium *tert*-butoxide completely. After the second portion of potassium *tert*-butoxide was added, the bottle was allowed to warm to 25° C. After 30 min. at 25° C, all the potassium *tert*-butoxide dissolved and the solutions had various dark colors. The phenoxide solution was added to the swollen resin in two portions, shaking between portions. The 1L bottles were clamped horizontally in an orbital shaker oven and allowed to shake at 25° C for 30 min. The temperature was then increased to 50° C and the reaction allowed to shake for 14 h. After cooling, each resin slurry was poured into a 8" x 10" 3-sided porous polypropylene packet (tea bag) sitting in a 2 L beaker. After the solvent mixture had drained from the resin, the fourth side of the tea bag was sealed and the tea bags were washed in wide-mouth HDPE Nalgene bottles as follows: 2 x DMF, 4 x DMF/H₂O (4:1), 3 x DMF, 4 x MeOH. The tea bags were allowed to air dry in a fume hood.

Step 1b. Loading Diamines on Wang-Imidazolid Resin

[0112] For each R₁ diamine, a 4 L Nalgene bottle was charged with 17 x 2.5 g

tea bags containing Wang resin (100-200 mesh, 1.4 mmol/g). DCM (2 L) was added followed by 1,1'-carbonyldiimidazole (97 g, 0.60 mol, 0.3 M). The bags were shaken for 3 h at room temperature. Each diamine (0.72 mol, 0.4 M) was placed in a 2 L Nalgene bottle and 1.8 L of DCM added.

[0113] After 3 h shaking with CDI, the Wang-imidazolidine tea bags were washed quickly with DCM (x2). The diamine solution was added immediately and the bags shaken overnight at room temperature. The bags were washed with DCM (x3) and MeOH (x3).

Step 2a. Imine Formation for the R₁ Hydroxybenzaldehydes.

[0114] After splitting the tea bags from step 1a, each set of 8 x 2.5 g bags was placed into a 1 L Nalgene bottle. The containers were then filled with 250 ml of trimethylorthoformate and 250 ml of anhydrous DMF. After the bags were saturated with the solvent, the primary amine (150 mmol, 0.3 M) was added. The reaction was then allowed to shake at room temperature for 24 h. The wash procedure must be carried out just before step 3 and the description is included in that section.

Step 2b. Imine Formation for the R₁ Primary Diamines.

[0115] After splitting the tea bags from step 1b, each set of 7 x 2.5 g bags was placed into a 1 L Nalgene bottle. The containers were then filled with 250 ml of trimethylorthoformate and 250 ml of anhydrous DMF. After the bags were saturated with the solvent, the aldehyde (150 mmol, 0.3 M) was added. The reaction was then shaken at room temperature for 24 h. The wash procedure must be carried out just before step 3 and is described in that section.

Step 3. Cyclization with 2-Phenylglutaric Anhydride

[0116] In an 8L Nalgene bottle, 2-Phenylglutaric anhydride (1.0 mol, 0.4M) was completely dissolved in 2.5L anhydrous DMF and triethylamine (0.03 M) was added. This anhydride solution is created before washing the imine tea bags. The imine tea bags from step 2 (60 X 2.5g bags) were quickly washed with

anhydrous DMF (3 x, 3 minutes or less washing). After washing, the imine bags were immediately transferred to the 2-Phenylglutaric anhydride solution and the reaction shaken at RT for 5 days. The bags were washed with DMF (x3) DCM (x3) and MeOH (x3) and air-dried.

Step 4. Acylation of the Resin Bound Carboxylic Acid.

[0117] Each tea bag from step 3 was plated into 40 wells of a 2 ml deep-well microtiter plate. The resin bound carboxylic acid was pre-activated by treatment with 0.6 ml of a solution containing 0.6 M DIC, 0.6M HOBt in anhydrous DMF. The plates were allowed to stand for one hour at room temperature. During this time, each amine solution was prepared by dissolving the amine (0.6M) in a solution of DIEA (0.8 M) in DMF. To each well containing the pre-activated acid resin was added 0.6 ml of the amine solution. The final concentrations in each well were: amine (0.3M), DIEA (0.4 M), HOBt (0.3 M), and DIC (0.3 M). The plates were vortexed and were placed in a shaker oven at 50° C for 24 h. After cooling to room temperature, the resin was washed using a robotic wash station with 20% water/DMF (x2), DMF (x8) and MeOH (x6) and air-dried.

Step 5. Cleavage from Linker and Extraction

[0118] To dry microtiter plates was added 0.5 ml of 20% TFA/DCM to each well. The plates were capped and placed on a shaker at room temperature for 2 h. The plates were transferred to a GENEVAC to remove the volatile TFA/DCM solution. The resin was extracted with AcOH and the extracts were frozen and lyophilized to afford the products as yellow oils. All of the final products were analyzed by HPLC/MS using ELSD detection to determine purity.

Example 2

Preparation of (Substituted Phenyl)-glutaric anhydrides

[0119] The appropriate substituted phenylacetic acid ethyl or methyl ester **1** (0.01 mol) is dissolved in anhydrous ethanol (100 ml). To this solution is added

Sodium ethoxide (0.01 mol), followed by ethyl acrylate (0.015 mol), and the solution is heated to reflux overnight. The solution is cooled and the solvent evaporated under reduced pressure. The product **2** is then dissolved in 100 ml H₂O/EtOH 1:1 and KOH added (0.10 mol). The solution is heated to reflux for 10 hours, acidified to pH 3 with 1 N HCl and the diacid product **3** extracted with EtOAc, washed with water and brine, and dried with MgSO₄. After removal of the solvent, the resulting solid is suspended in Acetic anhydride (100 ml) and heated to reflux for 1 hour to afford the anhydride. The solvent is removed and the residue is suspended in toluene and evaporated to afford the product **4**.

List of Compounds **1**:

ETHYL 2-THIOPHENEACETATE
 ETHYL THIOPHENE-3-ACETATE
 INDOLE-3-ACETIC ACID ETHYL ESTER
 ETHYL 2-PYRIDYLACETATE
 ETHYL 3-PYRIDYLACETATE
 ETHYL O-TOLYLACETATE
 ETHYL P-TOLYLACETATE
 METHYL 1-METHYL-2-PYRROLEACETATE
 METHYL 2,3,4,5,6-PENTAFLUOROPHENYLACETATE
 ETHYL 2-NAPHTHYLACETATE
 METHYL 2-(4,5-DIMETHOXY-2-NITROPHENYL)ACETATE
 ETHYL P-BROMOPHENYLACETATE
 ETHYL 4-NITROPHENYLACETATE
 METHYL 2,3,4-TRIMETHOXYPHENYL ACETATE
 METHYL 3,4,5-TRIMETHOXYPHENYL ACETATE
 ETHYL 3,4-DIMETHOXYPHENYLACETATE
 ETHYL M-TOLYLACETATE
 2,4-DICHLOROPHENYLACETIC ACID METHYL ESTER
 ETHYL 4-CHLOROPHENYLACETATE
 ETHYL 1-NAPHTHYLACETATE
 ETHYL 3-METHOXYPHENYLACETATE
 ETHYL 4-BENZYLOXYPHENYLACETATE
 ETHYL 4-METHOXYPHENYLACETATE
 5-BENZYLOXYINDOLE-3-ACETIC ACID METHYL ESTER
 ETHYL PYRIDINE-4-ACETATE
 METHYL 4-TERT-BUTYLPHENYLACETATE
 ETHYL MESITYLACETATE
 ETHYL 4-ETHOXYPHENYLACETATE
 ETHYL 2-BROMOPHENYLACETATE
 4-BUTOXYPHENYLACETIC ACID METHYL ESTER

ETHYL 3,5-DIMETHYLPHENYLACETATE
 METHYL 3,5-DIMETHOXYPHENYLACETATE
 ETHYL 2-NITROPHENYLACETATE
 2-CHLOROPHENYLACETIC ACID METHYL ESTER
 METHYL 4-BENZYLOXYPHENYLACETATE
 METHYL 5-CHLOROBENZO[B]THIEN-3-YLACETATE
 2,6-DICHLOROPHENYLACETIC ACID METHYL ESTER
 ETHYL 2,5-DIMETHOXYPHENYLACETATE
 METHYL (5-METHYL-2-PHENYLOXAZOL-4-YL)ACETATE
 METHYL 5,6-DICHLORO-3-INDOLEACETATE
 METHYL 2-(5-METHOXY-2-METHYL-1H-INDOL-3-YL)ACETATE
 METHYL (5-METHYL-2-PHENYLTHIAZOL-4-YL)ACETATE
 IMIDAZO(2,1-B)THIAZOL-6-YL-ACETIC ACID ETHYL ESTER
 (4-CHLORO-2-NITRO-PHENYL)-ACETIC ACID ETHYL ESTER
 ETHYL 2-(TRIFLUOROMETHYL)PHENYL ACETATE
 ETHYL 2-[2-(ACETYLAMINO)-1,3-THIAZOL-4-YL]ACETATE
 (1H-IMIDAZOL-4-YL)-ACETIC ACID METHYL ESTER
 (4,5-DIMETHOXY-2-NITRO-PHENYL)-ACETIC ACID ETHYL ESTER
 ETHYLFURYL ACETATE
 METHYL 2-FLUOROPHENYLACETATE
 METHYL 2-CHLORO-6-FLUOROPHENYLACETATE
 METHYL 4-FLUOROPHENYLACETATE
 METHYL 2-CHLORO-4-FLUOROPHENYL ACETATE
 METHYL 3-CHLOROPHENYLACETATE
 METHYL 3,4-DICHLOROPHENYLACETATE
 ETHYL 2-(2-PHENYL-1,3-THIAZOL-4-YL)ACETATE
 ETHYL 3,4-DICHLOROPHENYLACETATE
 ETHYL 2-(2-METHYL-1,3-THIAZOL-4-YL)ACETATE
 ETHYL 2-[2-[4-(TERT-BUTYL)PHENYL]-1,3-THIAZOL-4-YL]ACETATE
 ETHYL 2-[2-(4-CHLOROPHENYL)-1,3-THIAZOL-4-YL]ACETATE
 METHYL (2-CYANOPHENYL)ACETATE
 METHYL (4-CYANOPHENYL)ACETATE

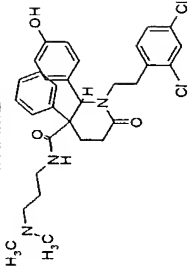
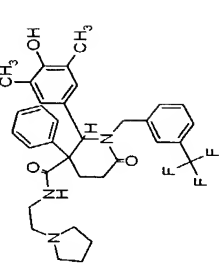

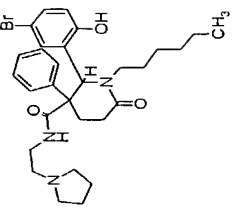
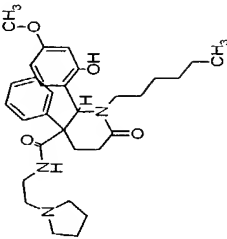
Example 3

Anti-microbial Screen

[0120] *Streptococcus pyogenes* (ATCC# 97-03 14289) was grown in Todd Hewitt Broth (THB) (Difco Laboratories #0492-17-6) overnight until reaching an optical density of (OD = 0.636@ 570 nm) by reading 0.1 ml in a 96 well microtiter plate in a Molecular Devices Thermomax. This preparation was kept frozen as stocks in 30% v/v glycerol in 1.5 ml aliquots at -70mC until use. Prior to experiments, 6 ml aliquots were thawed and diluted into 50 ml 2X THB. 60 ul

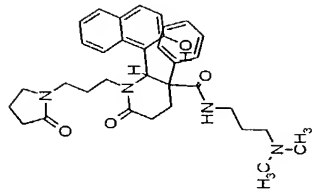
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37

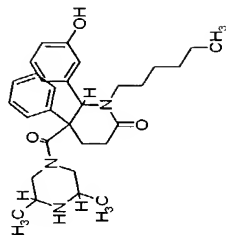
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9100	682	1	000726065	9100-009	B 07	0.112	Spy4H	98.90	0.1776	0.1776	TR0910000682				<chem>C34H38F3N3O3</chem>	593.686
9100	2442	1	000727585	9100-035	B 07	0.17	Spy4H	97.52	0.1776	0.1776	TR0910002442				<chem>C30H40BrN3O3</chem>	570.568
9100	3002	1	000728145	9100-042	B 07	0.112	Spy4H	97.51	0.1776	0.1776	TR0910003002				<chem>C31H43N3O4</chem>	521.698

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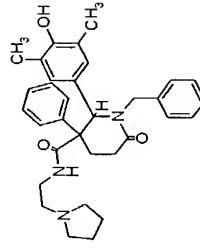
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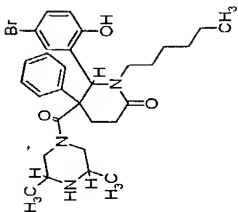
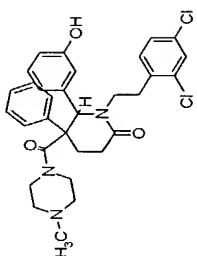
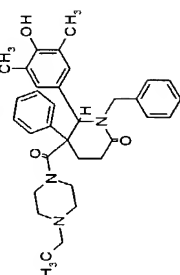
9100	1029	1	000726412	9100-013	E 10	0.162	94.11	Spy4H	0.1776	TR0910001029	#NAME?	C ₃₀ H ₄₁ N ₃ O ₃	491.672
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9100	2402	1	000727545	9100-035	B 02	0.12	92.38	Spy4H	0.1776	TR0910002402	#NAME?	C ₃₃ H ₃₉ N ₃ O ₃	525.689
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491.672 525.689

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?		
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9100	649	1	000726032	9100-009	A 03	0.217	84.40	Spy4H	0.1776	TR0910000649		#NAME?		C ₃₁ H ₃₃ Cl ₂ N ₃ O ₃ 566.526
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42

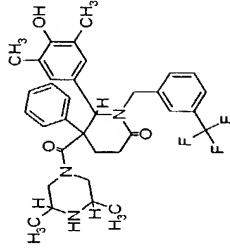
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593.686

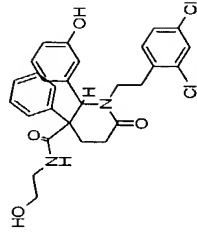


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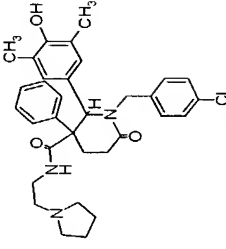


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560.134

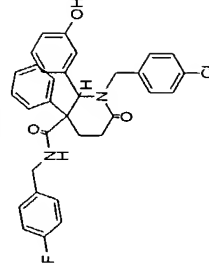


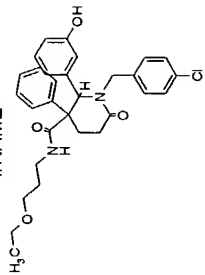
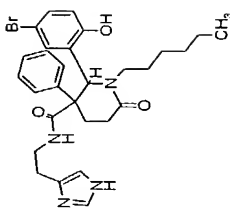
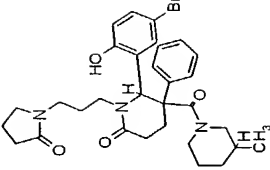
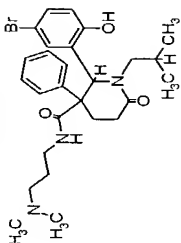
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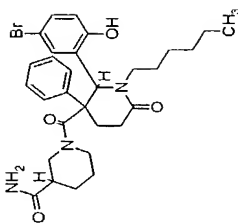
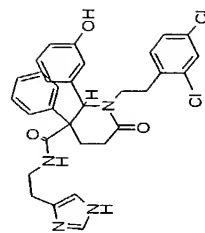
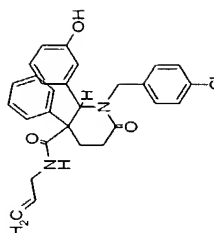
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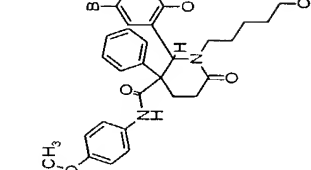
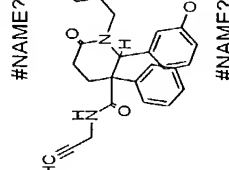
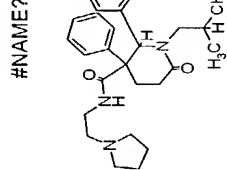
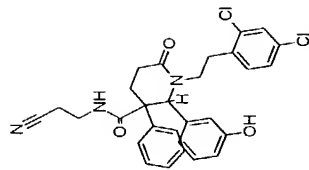
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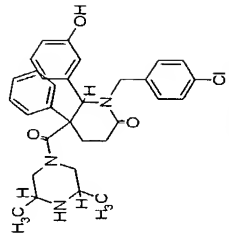
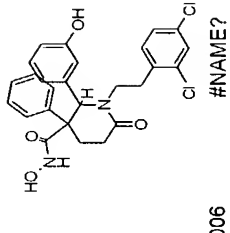
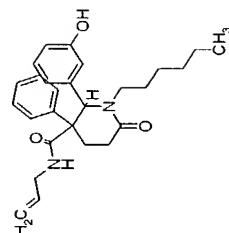
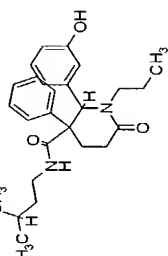
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9100	2444	1	000727587	9100-035	D 07	0.275	82.77	0.1776	0.1776	0.1776	0.1776	TR0910002444	C ₂₉ H ₃₅ Br N ₄ O ₃		C ₂₉ H ₃₅ Br N ₄ O ₃	567.524
9100	995	1	000726378	9100-013	C 06	0.291	82.45	0.1776	0.1776	0.1776	0.1776	TR0910000995	C ₃₁ H ₃₅ Br N ₃ O ₄		C ₃₁ H ₃₅ Br N ₃ O ₄	596.562
9100	1699	1	000726842	9100-023	C 04	0.177	82.26	0.1776	0.1776	0.1776	0.1776	TR0910001699	C ₂₇ H ₃₆ Br N ₃ O ₃		C ₂₇ H ₃₆ Br N ₃ O ₃	530.503

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C ₃₀ H ₃₈ Br N ₃ O ₄	584.551
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9100	644	1	000726027	9100-009	D 02	0.211	78.67	Spy4H	0.1776	TR0910000644		C ₃₁ H ₃₀ Cl ₂ N ₄ O ₃	577.509
9100	846	1	000726229	9100-011	F 07	0.31	78.13	Spy4H	0.1776	TR0910000846		C ₂₈ H ₂₇ Cl N ₂ O ₃	474.985

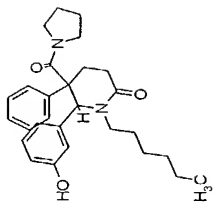
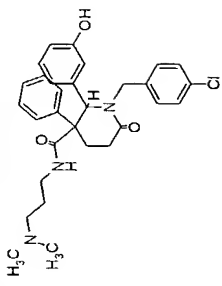
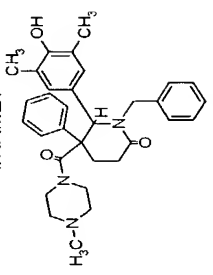
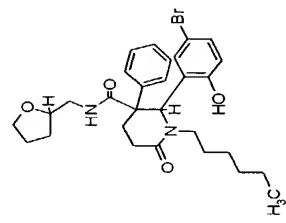
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9100	674	1	000726057	9100-009	B 06	0 275	77 32	Spy4H	0 1776	TR0910000674			
9100	1682	1	000726825	9100-023	B 02	0 193	77.18	Spy4H	0 1776	TR0910001682			
9100	870	1	000726253	9100-011	F 10	0 278	76 50	Spy4H	0 1776	TR0910000870			
9100	2476	1	000727619	9100-035	D 11	0 35	75.71	Spy4H	0 1776	TR0910002476			

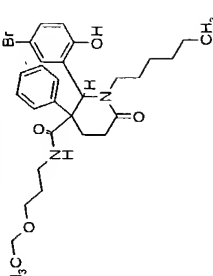
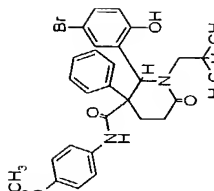
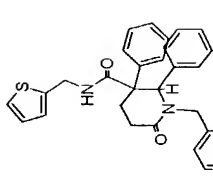
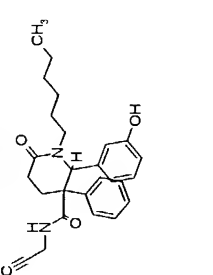


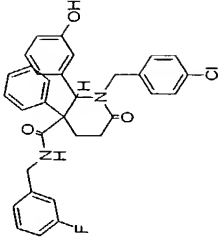
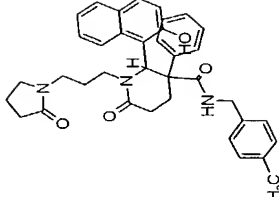
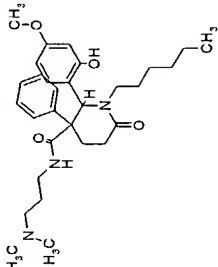
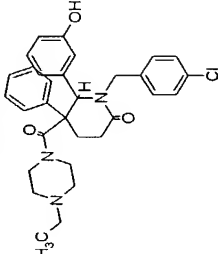
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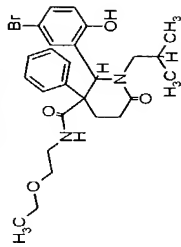
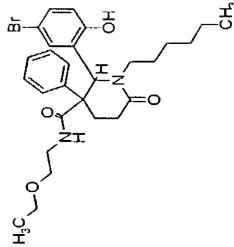
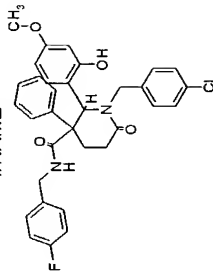
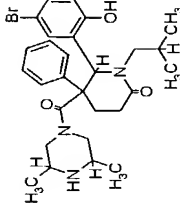
Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	$C_{31}H_{34}ClN_3O_3$	532.081
9100	869	1	000726252	9100-011	E 10	0.255	75.69	Spy4H	0.1776	TR0910000869					
9100	677	1	000726060	9100-009	E 06	0.23	75.63	Spy4H	0.1776	TR0910000677				$C_{26}H_{24}Cl_2N_2O_4$	499.392
9100	1006	1	000726389	9100-013	F 07	0.334	75.14	Spy4H	0.1776	TR0910001006				$C_{27}H_{34}N_2O_3$	434.577
9100	1101	1	000726484	9100-014	E 09	0.263	74.29	Spy4H	0.1776	TR0910001101				$C_{26}H_{34}N_2O_3$	422.566

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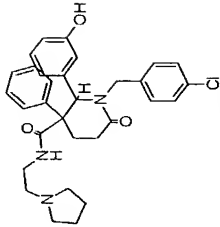
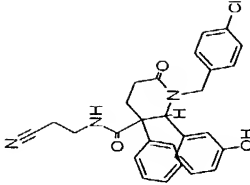
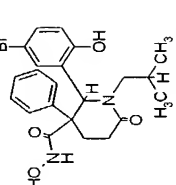
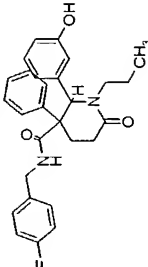
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	C ₂₈ H ₃₅ N ₂ O ₃	448 603
9100	1003	1	000726386	9100-013	C 07	0.302	74.05	Spy4H	0.1776	TR0910001003					
9100	859	1	000726242	9100-011	C 09	0.204	73.80	Spy4H	0.1776	TR0910000859				C ₃₀ H ₃₄ Cl N ₃ O ₃	520.07
9100	2409	1	000727552	9100-035	A 03	0.211	73.79	Spy4H	0.1776	TR0910002409				C ₃₂ H ₃₇ N ₃ O ₃	511.662
9100	2450	1	000727593	9100-035	B 08	0.294	73.79	Spy4H	0.1776	TR0910002450				C ₂₉ H ₃₇ Br N ₂ O ₄	557.525

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?	Chemical Structure	Molecular Formula	Mass
9100	2462	1	000727605	9100-035	F 09	0.254	73.79	Spy4H	0.1776	TR0910002462	TR0910002462	NAME?		C ₂₉ H ₃₉ Br N ₂ O ₄	559.541
9100	1716	1	000726859	9100-023	D 06	0.445	73.16	Spy4H	0.1776	TR0910001716	TR0910001716	NAME?		C ₂₉ H ₃₁ Br N ₂ O ₄	551.478
9100	858	1	000726241	9100-011	B 09	0.303	72.99	Spy4H	0.1776	TR0910000858	TR0910000858	NAME?		C ₃₀ H ₂₇ Cl N ₂ O ₃ S	531.073
9100	1030	1	000726413	9100-013	F 10	0.28	72.97	Spy4H	0.1776	TR0910001030	TR0910001030	NAME?		C ₂₇ H ₃₂ N ₂ O ₃	432.561

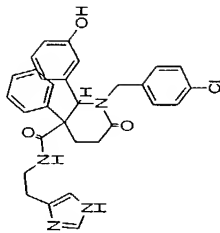
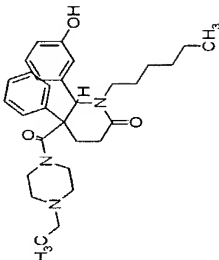
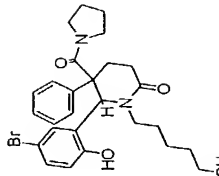
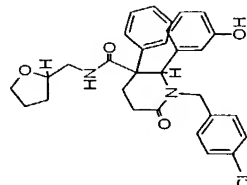
Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	Chemical Structure	Molecular Formula	Mass
9100	852	1	000726235	9100-011	D 08	0.332	72.45	Spy4H	0.1776	TR0910000852	#NAME?		C ₃₂ H ₂₈ Cl F N ₂ O ₃	543.035
9100	3731	1	000728874	9100-051	C 08	0.3	72.29	Spy4H	0.1776	TR0910003731	#NAME?		C ₃₇ H ₃₃ N ₃ O ₄	589.732
9100	3019	1	000728162	9100-042	C 09	0.205	72.18	Spy4H	0.1776	TR0910003019	#NAME?		C ₃₀ H ₄₃ N ₃ O ₄	509.687
9100	860	1	000726243	9100-011	D 09	0.266	72.18	Spy4H	0.1776	TR0910000860	#NAME?		C ₃₁ H ₃₄ Cl N ₃ O ₃	532.081

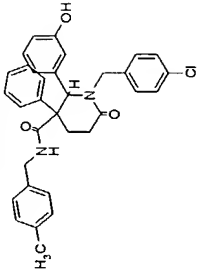
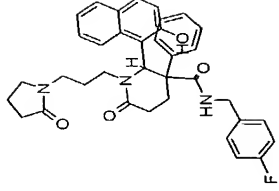
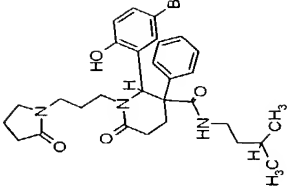
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?				
9100	1708	1	000726851	9100-023	D 05	0.379	72.09	Spy4H	0.1776	TR0910001708			C ₂₆ H ₃₃ Br N ₂ O ₄	517.461		
9100	2468	1	000727611	9100-035	D 10	0.28	71.54	Spy4H	0.1776	TR0910002468			C ₂₈ H ₃₇ Br N ₂ O ₄	545.514		
9100	2733	1	000727876	9100-039	E 03	0.429	71.19	Spy4H	0.1776	TR0910002733			C ₃₃ H ₃₀ Cl F N ₂ O ₄	573.061		
9100	1709	1	000726852	9100-023	E 05	0.383	71.02	Spy4H	0.1776	TR0910001709			C ₂₈ H ₃₆ Br N ₃ O ₃	542.514		

4064249 : 6646493

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?						
9100	842	1	000726225	9100-011	B 07	70.82	Spy4H	0.1776	70.82	0.1776	TR0910000842		C ₃₁ H ₃₄ Cl N ₃ O ₃	532.081				
9100	874	1	000726257	9100-011	B 11	70.82	Spy4H	0.1776	70.82	0.1776	TR0910000874		C ₂₈ H ₂₅ Cl N ₃ O ₃	487.984				
9100	1717	1	000726860	9100-023	E 06	70.21	Spy4H	0.1776	70.21	0.1776	TR0910001717		C ₂₂ H ₂₅ Br N ₂ O ₄	461.353				
9100	1093	1	000726476	9100-014	E 08	70.04	Spy4H	0.1776	70.04	0.1776	TR0910001093		C ₂₈ H ₂₉ F N ₂ O ₃	460.546				

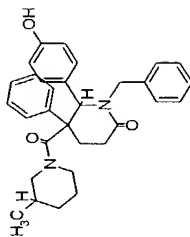
40949494 : 00949494

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc.mg/ml	LionID	#NAME?	C ₃₀ H ₂₉ Cl N ₄ O ₃	529.037
9100	844	1	000726227	9100-011	D 07	0.221	69.74	Spy4H	0.1776	TR0910000844				
9100	1020	1	000726403	9100-013	D 09	0.217	69.72	Spy4H	0.1776	TR0910001020			C ₃₀ H ₄₁ N ₃ O ₃	491.672
9100	2443	1	000727586	9100-035	C 07	0.383	69.62	Spy4H	0.1776	TR0910002443			C ₂₈ H ₃₅ Br N ₂ O ₃	527.5
9100	850	1	000726233	9100-011	B 08	0.322	69.47	Spy4H	0.1776	TR0910000850			C ₃₀ H ₃₁ Cl N ₂ O ₄	519.038

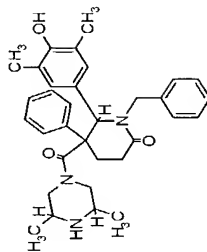
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	Chemical Structure	Molecular Formula	Mass
9100	851	1	000726234	9100-011	C 08	0 374	69 20	Spy4H	0 1776	TR0910000851			C ₃₃ H ₃₁ Cl N ₂ O ₃	539.072
9100	3733	1	000728876	9100-051	E 08	0 332	68 93	Spy4H	0 1776	TR0910003733			C ₃₅ H ₃₆ F N ₃ O ₄	593.595
9100	981	1	000726364	9100-013	E 04	0 321	68 63	Spy4H	0 1776	TR0910000981			C ₃₀ H ₃₃ Br N ₃ O ₄	584.551

Library Cmpd Lot ExpReg Plate Well Raw Data Assay Result Assay Conc mg/ml LionID

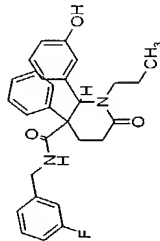
9100 1755 1 000726898 9100-023 C 11 0 363 67 80 Spy4H 0 1776 TR0910001755 #NAME? C₃₁ H₃₄ N₂ O₃ 482.621



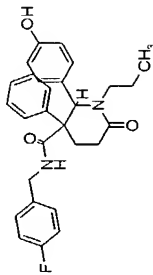
9100 2429 1 000727572 9100-035 E 05 0 217 67 70 Spy4H 0 1776 TR0910002429 #NAME? C₃₃ H₃₉ N₃ O₃ 525.689



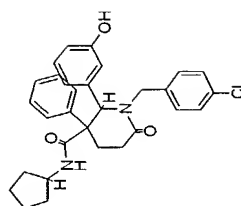
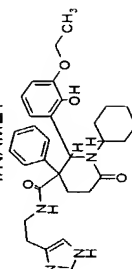
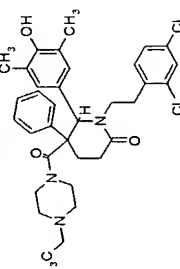
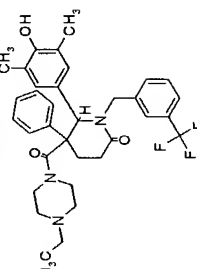
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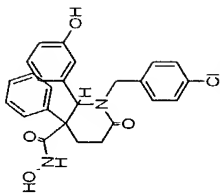
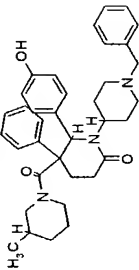
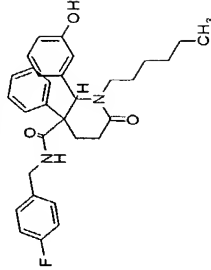
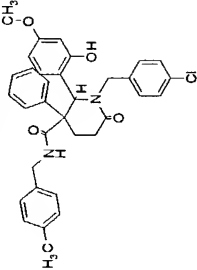
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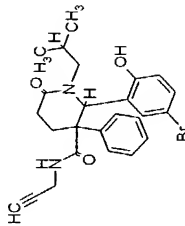
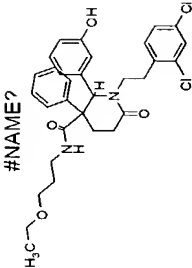
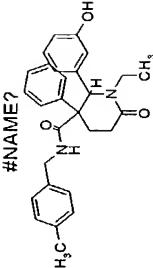
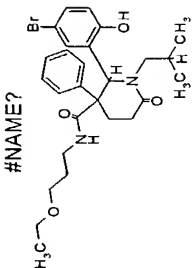
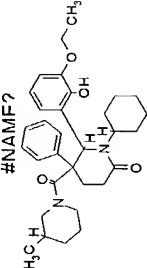
482.621 525.689 460.546 460.546

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc,mg/ml	LionID	#NAME?	C ₃₀ H ₃₁ Cl N ₂ O ₃	503 039	
9100	845	1	000726228	9100-011	E 07	0.421	67.31	Spy4H	0.1776	TR0910000845				
9100	2324	1	000727467	9100-033	D 02	0.232	66.94	Spy4H	0.1776	TR0910002324		#NAME?	C ₃₁ H ₃₈ N ₄ O ₄	530 665
9100	2500	1	000727643	9100-036	D 04	0.368	66.93	Spy4H	0.1776	TR0910002500		#NAME?	C ₃₄ H ₃₉ Cl ₂ N ₃ O ₃	608.606
9100	700	1	000726083	9100-009	D 09	0.288	66.86	Spy4H	0.1776	TR0910000700		#NAME?	C ₃₄ H ₃₈ F ₃ N ₃ O ₃	593 686

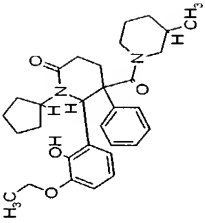
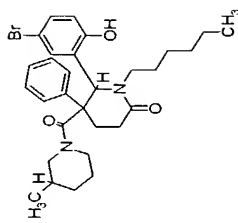
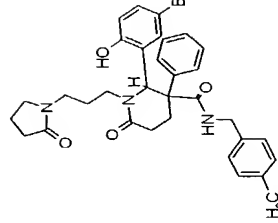
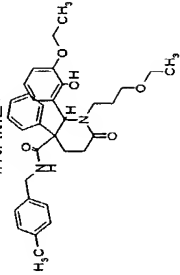
10094503 # 0020303

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	C ₂₈ H ₂₃ Cl N ₂ O ₄	450.92
9100	877	1	000726260	9100-011	E 11	0.255	66.77	Spy4H	0.1776	TR0910000877					
9100	2595	1	0007272738	9100-037	C 06	0.24	66.62	Spy4H	0.1776	TR0910002595				C ₃₈ H ₄₃ N ₃ O ₃	565 754
9100	1013	1	000726396	9100-013	E 08	0.414	66.46	Spy4H	0.1776	TR0910001013				C ₃₁ H ₃₅ F N ₂ O ₃	502 626
9100	2731	1	000727874	9100-039	C 03	0.388	66.26	Spy4H	0.1776	TR0910002731				C ₃₄ H ₃₃ Cl N ₂ O ₄	569 098

60

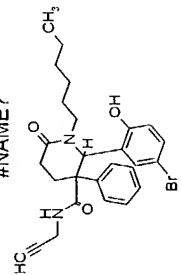
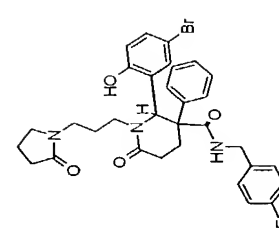
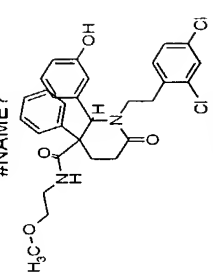
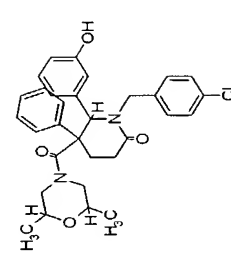
Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C ₂₅ H ₂₇ Br N ₂ O ₃	483.403
9100	1710	1	000726853	9100-023	F 05	0.415	66.20	Spy4H	0.1776	TR0910001710			
9100	662	1	000726045	9100-009	F 04	0.32	65.85	Spy4H	0.1776	TR0910000662		569.526	
9100	731	1	000726114	9100-010	C 03	0.283	65.76	Spy4H	0.1776	TR0910000731		442.556	
9100	1702	1	000726845	9100-023	F 04	0.417	65.66	Spy4H	0.1776	TR0910001702		531.487	
9100	2355	1	000727498	9100-033	C 06	0.452	65.53	Spy4H	0.1776	TR0910002355		518.694	

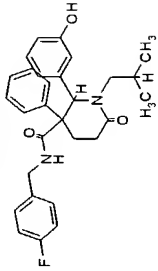
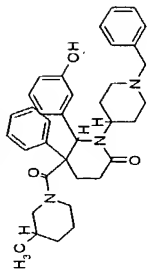
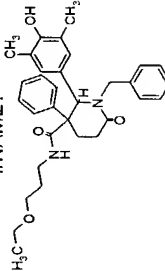
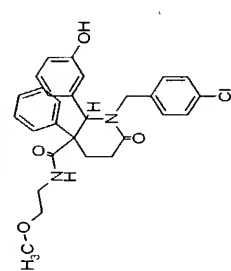
483.403 569.526 442.556 531.487 518.694

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	C ₃₁ H ₄₀ N ₂ O ₄	504 667
9100	1955	1	000727098	9100-028	C 06	0 353	65.27	Spy4H	0 1776	TR0910001955					
9100	2475	1	000727618	9100-035	C 11	0 305	65 13	Spy4H	0 1776	TR0910002475				C ₃₀ H ₃₉ Br N ₂ O ₃	555 553
9100	971	1	000726354	9100-013	C 03	0 379	65.11	Spy4H	0 1776	TR0910000971				C ₃₃ H ₃₆ Br N ₃ O ₄	618 568
9100	2531	1	000727674	9100-036	C 08	0 302	65.06	Spy4H	0 1776	TR0910002531				C ₃₃ H ₄₀ N ₂ O ₅	544 688

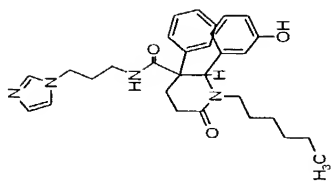
40091955 # 555553

Library	Cmpd	Lot	ExReg	Plate	Well	RawData	Assay	Result	Assay	Conc	mg/ml	LionID
9100	2533	1	000727676	9100-036	E 08	0.304	Spy4H	65.06	0.1776	0.1776	TR0910002533	
<div> <div>#NAME?</div> <div> <chem>CCOC(=O)NCCC1c2cc(F)ccc2C(=O)N1C3C(O)c4ccccc4O3</chem> </div> <div>C₃₂ H₃₇ F N₂ O₅</div> <div>548.651</div> </div>												
9100	843	1	000726226	9100-011	C 07	0.364	Spy4H	64.87	0.1776	0.1776	TR0910000843	
<div> <div>#NAME?</div> <div> <chem>CCOC(=O)NCCC1c2cc(O)ccc2C(=O)N1C3C(O)c4ccccc4O3</chem> </div> <div>C₂₉ H₂₉ Cl N₂ O₃</div> <div>489.012</div> </div>												
9100	2740	1	000727883	9100-039	D 04	0.384	Spy4H	64.80	0.1776	0.1776	TR0910002740	
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9100	612	1	000725995	9100-008	D 08	0.339	Spy4H	64.80	0.1776	0.1776	TR0910000612	
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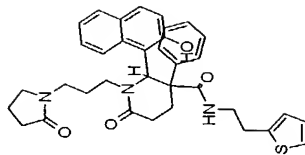
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID			
9100	2470	1	000727613	9100-035	F 10	0.294	64.49	Spy4H	0.1776	TR0910002470	#NAME?		C ₂₇ H ₃₁ Br N ₂ O ₃	511.457
9100	973	1	000726356	9100-013	E 03	0.304	64.02	Spy4H	0.1776	TR0910000973	#NAME?		C ₃₂ H ₃₃ Br F N ₃ O ₄	622.532
9100	647	1	000726030	9100-009	G 02	0.295	63.83	Spy4H	0.1776	TR0910000647	#NAME?		C ₂₉ H ₃₀ Cl ₂ N ₂ O ₄	541.472
9100	878	1	000726261	9100-011	F 11	0.356	63.79	Spy4H	0.1776	TR0910000878	#NAME?		C ₃₁ H ₃₃ Cl N ₂ O ₄	533.065

Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	Chemical Structure	Molecular Formula	Mass
9100	573	1	000725956	9100-008	E 03	0.359	63.64	Spy4H	0.1776	TR0910000573	TR0910000573	474.573	<chem>C29H31FN2O3</chem>		<chem>C29H31FN2O3</chem>	474.573
9100	2235	1	000727378	9100-031	C 11	0.239	63.59	Spy4H	0.1776	TR0910002235	TR0910002235	565.754	<chem>C36H43N3O3</chem>		<chem>C36H43N3O3</chem>	565.754
9100	2422	1	000727565	9100-035	F 04	0.259	63.53	Spy4H	0.1776	TR0910002422	TR0910002422	514.662	<chem>C32H38N2O4</chem>		<chem>C32H38N2O4</chem>	514.662
9100	847	1	000726230	9100-011	G 07	0.292	63.52	Spy4H	0.1776	TR0910000847	TR0910000847	493	<chem>C28H28ClN2O4</chem>		<chem>C28H28ClN2O4</chem>	493

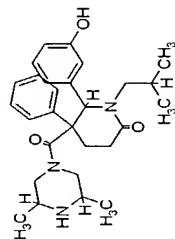
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C ₃₀ H ₃₈ N ₄ O ₃	502.655
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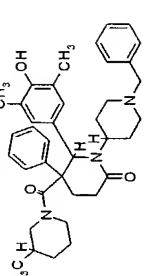
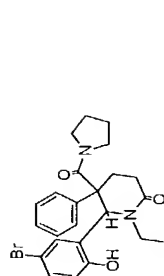
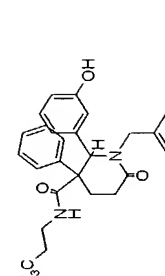
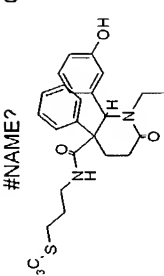


9100	3751	1	000728894	9100-051	G 10	0.289	63.44	Spy4H	0.1776	TR0910003751	#NAME?	C ₃₅ H ₃₇ N ₃ O ₄ S	595.76
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9100	589	1	000725972	9100-008	E 05	0.225	63.35	Spy4H	0.1776	TR0910000589	#NAME?	C ₂₈ H ₃₇ N ₃ O ₃	463.618
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Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?			
9100	4155	1	000729298	9100-057	C 11	0.321	63.27	Spy4H	0.1776	0.1776	TR0910004155		#NAME?		C ₃₉ H ₄₇ N ₃ O ₃	593.807
9100	1683	1	000726826	9100-023	C 02	0.484	63.25	Spy4H	0.1776	0.1776	TR0910001683		#NAME?		C ₂₅ H ₃₁ Br N ₂ O ₃	499.446
9100	856	1	000726239	9100-011	H 08	0.335	63.25	Spy4H	0.1776	0.1776	TR0910000856		#NAME?		C ₂₉ H ₂₉ Cl N ₂ O ₃	477.001
9100	865	1	000726248	9100-011	A 10	0.272	63.25	Spy4H	0.1776	0.1776	TR0910000865		#NAME?		C ₂₉ H ₃₁ Cl N ₂ O ₃ S	523.094

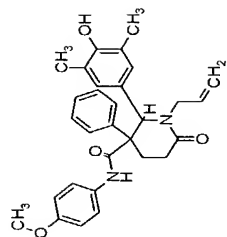
HOPE-2020-09-09

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID
9100	1076	1	000726459	9100-014	D 06	0.291	63.24	Spy4H	0.1776	0.1776		TR0910001076

C₃₀ H₃₂ N₂ O₄

#NAME?

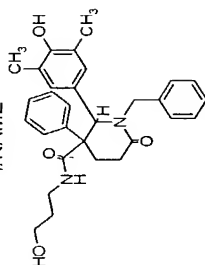
484.593



C₃₀ H₃₄ N₂ O₄

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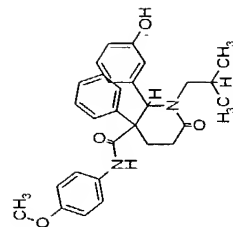
486.609



C₂₉ H₃₂ N₂ O₄

#NAME?

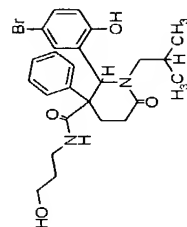
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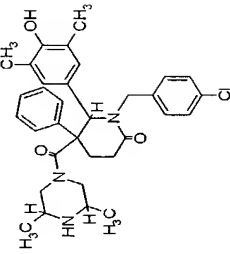
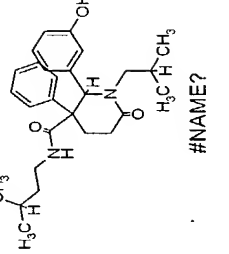
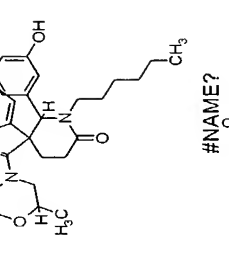
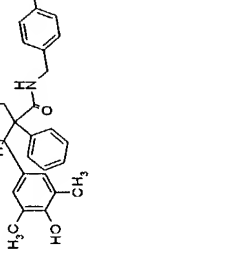


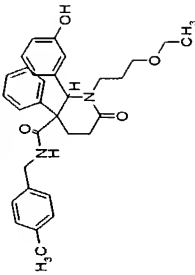
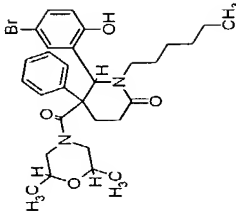
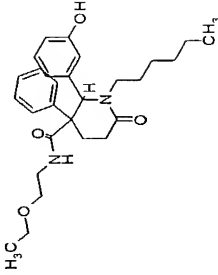
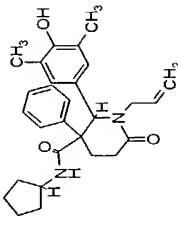
C₂₅ H₃₁ Br N₂ O₄

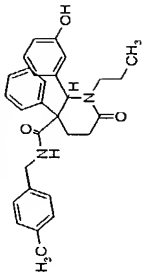
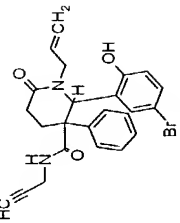
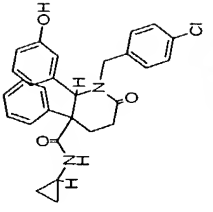
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503.434

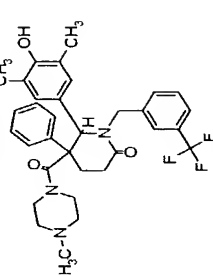
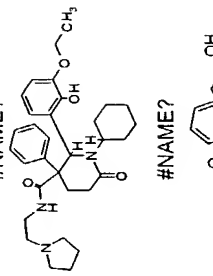
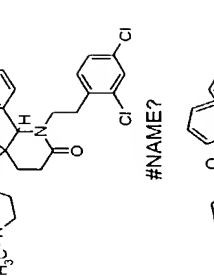
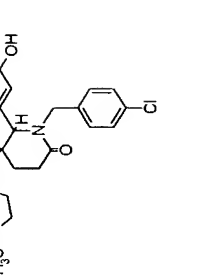


Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	Chemical Structure	Molecular Formula	Mass
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9100	581	1	000725964	9100-008	E 04	0.326	62.77	Spy4H	0.1776	TR0910000581			C ₂₇ H ₃₆ N ₂ O ₃	436.592
9100	1038	1	000726421	9100-013	F 11	0.295	62.40	Spy4H	0.1776	TR0910001038			C ₃₀ H ₄₀ N ₂ O ₄	492.656
9100	773	1	000726156	9100-010	E 08	0.231	62.39	Spy4H	0.1776	TR0910000773			C ₃₀ H ₃₁ FN ₂ O ₃	486.584

Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID		
9100	1971	1	000727114	9100-028	C 08	0.296	61.99	Spy4H	0.1776	TR0910001971		#NAME?	C ₃₁ H ₃₈ N ₂ O ₄ 500.635
													
9100	2478	1	000727621	9100-035	F 11	0.265	61.92	Spy4H	0.1776	TR0910002478		#NAME?	C ₃₀ H ₃₉ Br N ₂ O ₄ 571.552
													
9100	1028	1	000726411	9100-013	D 10	0.257	61.86	Spy4H	0.1776	TR0910001028		#NAME?	C ₂₈ H ₃₈ N ₂ O ₄ 466.618
													
9100	1045	1	000726428	9100-014	E 02	0.331	61.83	Spy4H	0.1776	TR0910001045		#NAME?	C ₂₈ H ₃₄ N ₂ O ₃ 446.588
													

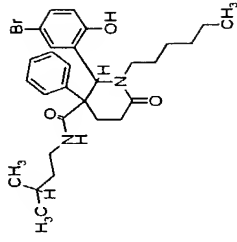
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?			
9100	1091	1	000726474	9100-014	C 08	0 346	61.83	Sp4H	0 1776	TR0910001091	456.583	C ₂₈ H ₃₂ N ₂ O ₃				
9100	230	1	000725613	9100-003	F 10	0 323	61.69	Sp4H	0 1776	TR091000230	467.361	C ₂₄ H ₂₃ Br N ₂ O ₃				
9100	855	1	000726238	9100-011	G 08	0 344	61.63	Sp4H	0 1776	TR091000855	474.985	C ₂₈ H ₂₇ Cl N ₂ O ₃				
9100	3741	1	000728884	9100-051	E 09	0 246	61.60	Sp4H	0 1776	TR0910003741	555.715	C ₃₄ H ₄₁ N ₃ O ₄				

9100 1091 1 000726474 9100-014 C 08 0 346 61.83 Sp4H 0 1776 TR0910001091 456.583 C₂₈ H₃₂ N₂ O₃

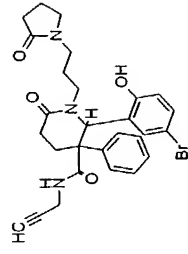
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc	mg/ml	LionID	
9100	689	1	000726072	9100-009	A 08	0.249	60.79	Spy4H	0.1776	TR0910000689	C ₃₃ H ₃₆ F ₃ N ₃ O ₃	579.659
<div> <div>#NAME?</div>  </div>												
9100	2322	1	000727465	9100-033	B 02	0.255	60.75	Spy4H	0.1776	TR0910002322	C ₃₂ H ₄₃ N ₃ O ₄	533.709
<div> <div>#NAME?</div>  </div>												
9100	2969	1	000728112	9100-042	A 03	0.328	60.74	Spy4H	0.1776	TR0910002969	C ₃₁ H ₃₃ Cl ₂ N ₃ O ₃	566.526
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9100	849	1	000726232	9100-011	A 08	0.295	60.55	Spy4H	0.1776	TR0910000849	C ₃₀ H ₃₂ Cl N ₃ O ₃	518.054
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10094545 - 000302

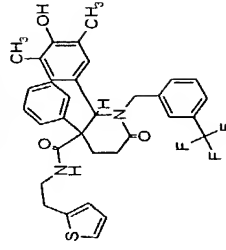
Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C ₂₉ H ₃₉ Br N ₂ O ₃	543.542
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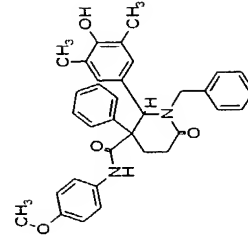
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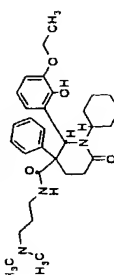
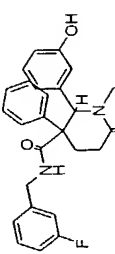
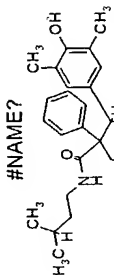
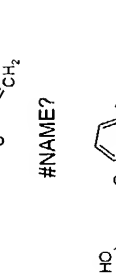
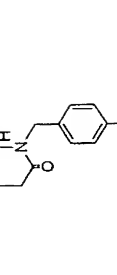


9100	711	1	000726094	9100-009	G 10	0.388	60.12	Spy4H	0.1776	TR0910000711	#NAME?	C ₃₄ H ₃₃ F ₃ N ₂ O ₃ S	606.706
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9100	2436	1	000727579	9100-035	D 06	0.314	60.00	Spy4H	0.1776	TR0910002436	#NAME?	C ₃₄ H ₃₄ N ₂ O ₄	534.653
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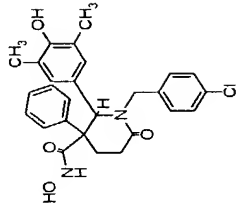


Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc.mg/ml	LionID	#NAME?		
9100	2339	1	000727482	9100-033	C 04	0.257	59.91	Spy4H	0.1776	TR0910002339		C ₃₁ H ₄₃ N ₃ O ₄	521.698
9100	572	1	000725955	9100-008	D 03	0.338	59.88	Spy4H	0.1776	TR0910000572		C ₂₉ H ₃₁ F N ₂ O ₃	474.573
9100	1061	1	000726444	9100-014	E 04	0.403	59.84	Spy4H	0.1776	TR0910001061		C ₂₉ H ₃₆ N ₂ O ₃	448.603
9100	857	1	000726240	9100-011	A 09	0.265	59.74	Spy4H	0.1776	TR0910000857		C ₂₇ H ₂₇ Cl N ₂ O ₄	478.973
9100	861	1	000726244	9100-011	E 09	0.427	59.74	Spy4H	0.1776	TR0910000861		C ₃₀ H ₃₃ Cl N ₂ O ₃	505.055

Library	Compd	Lol	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID
9100	2637	1	000727780	9100-037	E 11	0.35	59.73	Spy4H	0.1776	0.1776		TR0910002637

C₂₇ H₂₇ Cl N₂ O₄ 478.973

#NAME?



C₃₂ H₃₄ Br N₃ O₅ 620.541

TR0910000996

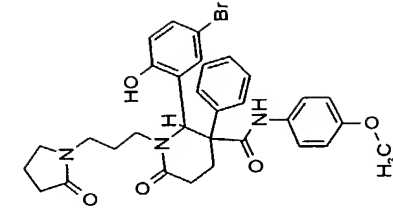
Spy4H 0.1776

59.69

0.279

D 06

9100 996 1 000726379 9100-013



C₂₈ H₃₈ Br N₃ O₃ 542.514

TR0910001700

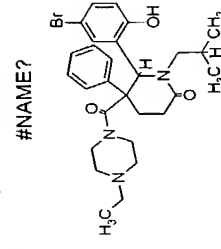
Spy4H 0.1776

59.50

0.316

D 04

9100 1700 1 000726843 9100-023

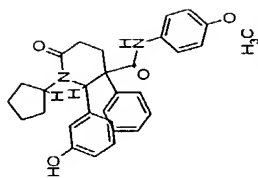


#NAME?

Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc (mg/ml)	LionID
9100	813	1	000726196	9100-011	E 03	0.38	59.47	Spy4H	0.1776	TR0910000813
<div> <div>#NAME?</div> <div> <chem>CCOCNCCC(=O)N1Cc2cc(F)ccc2C1=O</chem> </div> <div> <chem>COc1cc(O)c2c(c1)C(=O)N(CCCOCC)CC2=O</chem> </div> </div> <div> $C_{31}H_{35}FN_2O_5$ </div> <div>534.625</div>										
9100	2489	1	000727632	9100-036	A 03	0.361	59.45	Spy4H	0.1776	TR0910002489
<div> <div>#NAME?</div> <div> <chem>CC1CN(C1)C2Cc3cc(O)c(C)c3C2=O</chem> </div> <div> <chem>Clc1ccc(CCN2C(=O)N(CCC3Cc4cc(O)c(C)c4C3=O)CC2=O)cc1</chem> </div> </div> <div> $C_{33}H_{37}Cl_2N_3O_3$ </div> <div>594.579</div>										
9100	988	1	000726371	9100-013	D 05	0.247	59.42	Spy4H	0.1776	TR0910000988
<div> <div>#NAME?</div> <div> <chem>CCOCNCCC(=O)N1Cc2cc(O)c3c2C(=O)N(CCC4Cc5cc(Br)ccc5C4=O)CC1=O</chem> </div> <div> <chem>CCOCNCCC(=O)N1Cc2cc(O)c3c2C(=O)N(CCC4Cc5cc(Br)ccc5C4=O)CC1=O</chem> </div> </div> <div> $C_{29}H_{38}BrN_3O_5$ </div> <div>586.523</div>										

Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	IonID
9100	3236	1	000728379	9100-045	D 06	0 304	59 42	Spy4H	0 1776	TR0910003236	#NAME?	C ₃₀ H ₃₂ N ₂ O ₄

484.593



526.673

C₃₃ H₃₈ N₂ O₄

#NAME?

TR0910002438

0 1776

Spy4H

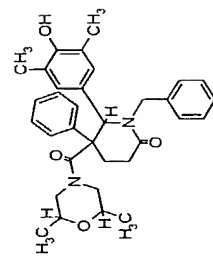
59 36

0 285

F 06

2438

9100



434.577

C₂₇ H₃₄ N₂ O₃

#NAME?

TR0910001115

0 1776

Spy4H

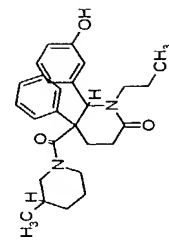
59 28

0 262

C 11

1115

9100



515.489

C₂₇ H₃₅ Br N₂ O₃

#NAME?

TR0910001701

0 1776

Spy4H

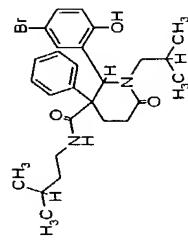
59 24

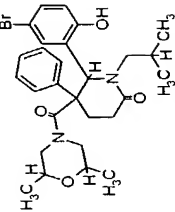
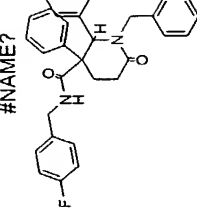
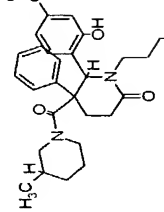
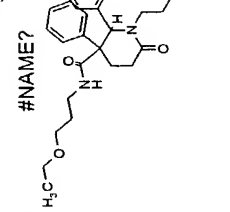
0 512

E 04

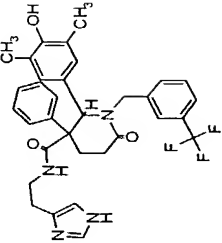
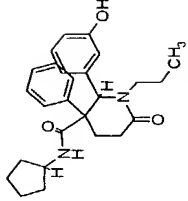
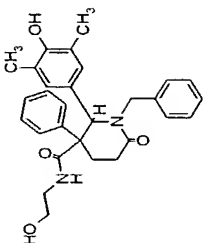
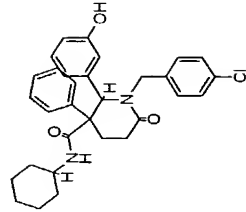
1701

9100

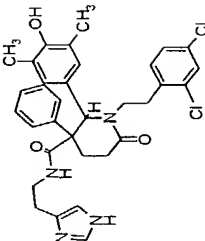
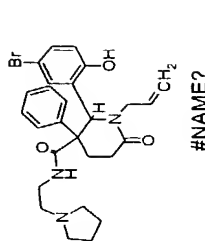
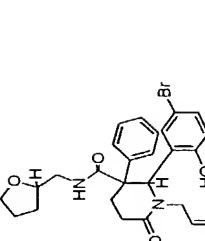



Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C ₂₈ H ₃₅ Br N ₂ O ₄	543 498
9100	1718	1	000726861	9100-023	F 06	0 364	59 24	Spy4H	0 1776	TR0910001718			
9100	1733	1	000726876	9100-023	E 08	0 331	59 24	Spy4H	0 1776	TR0910001733		C ₃₂ H ₂₉ F N ₂ O ₃	508 59
9100	835	1	000726218	9100-011	C 06	0 321	59 20	Spy4H	0 1776	TR0910000835		C ₃₀ H ₄₀ N ₂ O ₅	508 655
9100	1022	1	000726405	9100-013	F 09	0 261	59 15	Spy4H	0 1776	TR0910001022		C ₂₉ H ₄₀ N ₂ O ₄	480 645

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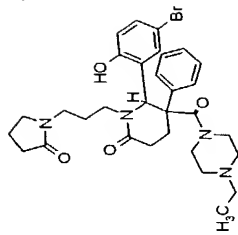
Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc (ng/ml)	LionID	#NAME?	Chemical Structure	Molecular Formula	Mass
9100	584	1	000726067	9100-009	D 07	0.231	58.43	Spy4H	0.1776	TR0910000684	#NAME?		C ₃₃ H ₃₃ F ₃ N ₄ O ₃	590.543
9100	1085	1	000726468	9100-014	E 07	0.26	58.43	Spy4H	0.1776	TR0910001085	#NAME?		C ₂₆ H ₃₂ N ₂ O ₃	420.55
9100	2417	1	000727560	9100-035	A 04	0.302	58.40	Spy4H	0.1776	TR0910002417	#NAME?		C ₂₉ H ₃₂ N ₂ O ₄	472.582
9100	848	1	000726231	9100-011	H 07	0.279	58.38	Spy4H	0.1776	TR0910000848	#NAME?		C ₃₁ H ₃₃ ClN ₂ O ₃	517.066

11/20/2019 10:00:00 AM

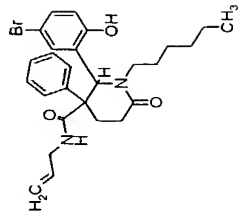
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?	C ₃₃ H ₃₄ Cl ₂ N ₄ O ₃	605.563
9100	2484	1	000727627	9100-036	D 02	0 319	58 38	Spy4H	0 1776	TR0910002484				
9100	202	1	000725585	9100-003	B 07	0 243	58 34	Spy4H	0 1776	TR0910000202			526.472	
9100	210	1	000725593	9100-003	B 08	0 331	58 34	Spy4H	0 1776	TR0910000210			513.429	
9100	3029	1	000728172	9100-042	E 10	0 279	58 29	Spy4H	0 1776	TR0910003029			521.698	

4024563 = 605.563

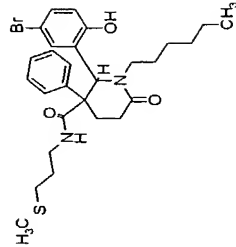
Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C ₂₁ H ₃₃ Br N ₄ O ₄	611.577
9100	980	1	000726363	9100-013	D 04	0.254	58.06	Spy4H	0.1776	TR0910000980			



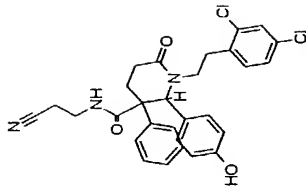
9100	2446	1	000727589	9100-035	F 07	0.408	57.76	Spy4H	0.1776	TR0910002446	#NAME?	C ₂₇ H ₃₃ Br N ₂ O ₃	513.473
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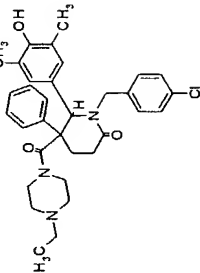
9100	2465	1	000727608	9100-035	A 10	0.25	57.76	Spy4H	0.1776	TR0910002465	#NAME?	C ₂₈ H ₃₇ Br N ₂ O ₃ S	561.581
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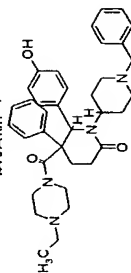
Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc	mg/ml	LionID	#NAME?	C ₂₉ H ₂₇ Cl ₂ N ₃ O ₃	536.456
9100	2994	1	000728137	9100-042	B 06	0.413	57.20	Spy4H	0.1776		TR0910002994			



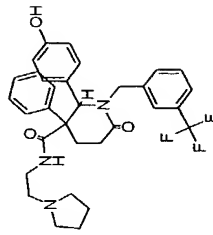
9100	2620	1	000727763	9100-037	D 09	0.268	57.14	Spy4H	0.1776		TR0910002620	#NAME?	C ₃₃ H ₃₈ Cl N ₃ O ₃	560.134
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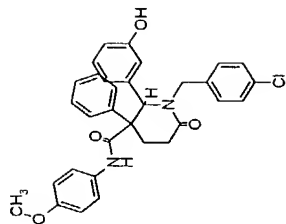
9100	2580	1	000727723	9100-037	D 04	0.243	56.86	Spy4H	0.1776		TR0910002580	#NAME?	C ₃₆ H ₄₄ N ₄ O ₃	580.769
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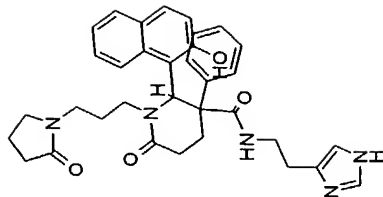
9100	4082	1	000729225	9100-057	B 02	0.248	56.80	Spy4H	0.1776		TR0910004082	#NAME?	C ₃₂ H ₃₄ F ₃ N ₃ O ₃	565.633
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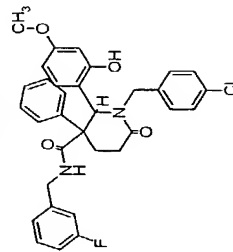
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc.mg/ml	LionID	#NAME?	C ₃₂ H ₂₉ Cl N ₂ O ₄	541 044
9100	876	1	000726259	9100-011	D 11	0.432	56.76	Spy4H	0.1776	TR0910000876			

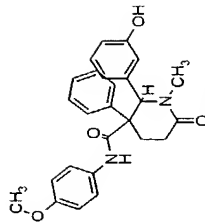
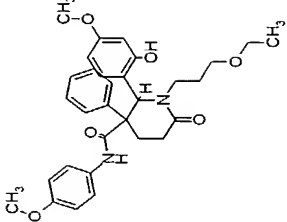
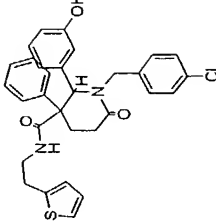


9100	3724	1	000728867	9100-051	D 07	0.252	56.72	Spy4H	0.1776	TR0910003724		C ₃₄ H ₃₇ N ₅ O ₄	579.697
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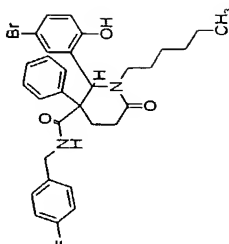
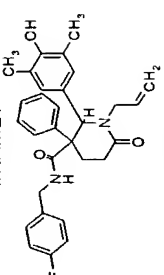
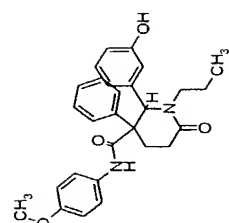
9100	2732	1	000727875	9100-039	D 03	0.457	56.68	Spy4H	0.1776	TR0910002732		C ₃₃ H ₃₀ Cl F N ₂ O ₄	573 061
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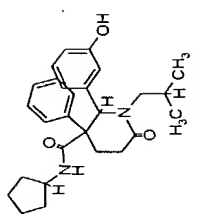
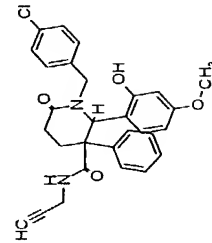
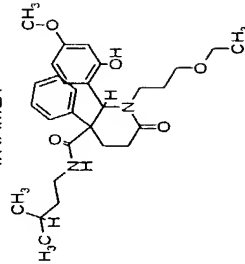
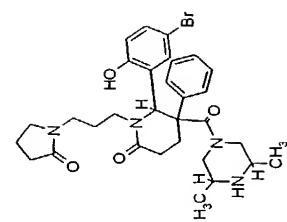
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	C ₂₆ H ₂₆ N ₂ O ₄	430.501
9100	196	1	000725579	9100-003	D 06	0 252	56 51	Spy4H	0 1776	TR0910000196					
9100	836	1	000726219	9100-011	D 06	0 304	56 49	Spy4H	0 1776	TR0910000836					
9100	871	1	000726254	9100-011	G 10	0 336	56 49	Spy4H	0 1776	TR0910000871					

9100 871 1 000726254 9100-011 G 10 0 336 56 49 Spy4H 0 1776 TR0910000871 C₃₁ H₂₈ Cl N₂ O₃ S 545 1

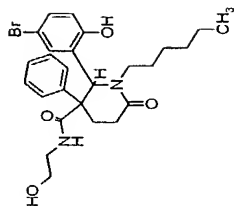
10094355 . 020322

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc (ng/ml)	LionID	#NAME?	C ₃₁ H ₃₄ Br F N ₂ O ₃	581.523
9100	2453	1	000727596	9100-035	E 08	0.43	56.47	Spy4H	0.1776	TR0910002453			
9100	1053	1	000726436	9100-014	E 03	0.478	56.44	Spy4H	0.1776	TR0910001053		C ₃₀ H ₃₁ F N ₂ O ₃	486.584
9100	1116	1	000726499	9100-014	D 11	0.265	56.44	Spy4H	0.1776	TR0910001116		C ₂₈ H ₃₀ N ₂ O ₄	458.555
9100	997	1	000726380	9100-013	E 06	0.254	56.44	Spy4H	0.1776	TR0910000997		C ₂₅ H ₂₈ Br N ₃ O ₅	530.416

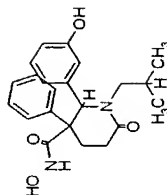
9100 2453 1 000727596 9100-035 E 08 0.43 56.47 Spy4H 0.1776 TR0910002453

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc.mg/ml	LionID	#NAME?	C ₂₇ H ₃₄ N ₂ O ₃	434.577
9100	565	1	000725948	9100-008	E 02	0 304	56.40	Spy4H	0 1776	TR0910000565			
9100	2750	1	000727893	9100-039	F 05	0 457	56.39	Spy4H	0 1776	TR0910002750		C ₂₉ H ₂₇ Cl N ₂ O ₄	502.995
9100	821	1	000726204	9100-011	E 04	0 322	56.22	Spy4H	0 1776	TR0910000821		C ₂₉ H ₄₀ N ₂ O ₅	496.644
9100	989	1	000726372	9100-013	E 05	0 257	56.17	Spy4H	0 1776	TR0910000989		C ₃₁ H ₃₉ Br N ₄ O ₄	611.577

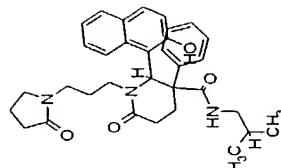
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C ₂₆ H ₃₃ Br N ₂ O ₄	517.461
9100	2457	1	000727600	9100-035	A 09	0 275	56 15	Spy4H	0 1776	TR0910002457			



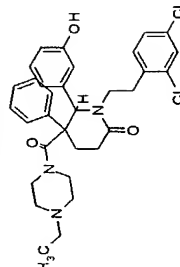
9100	597	1	000725980	9100-008	E 06	0 25	56.11	Spy4H	0 1776	TR0910000597	#NAME?	C ₂₂ H ₂₆ N ₂ O ₄	382.457
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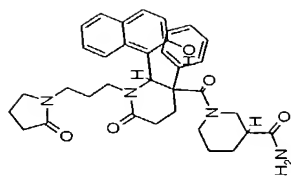
9100	3746	1	000728889	9100-051	B 10	0 268	56.11	Spy4H	0 1776	TR0910003746	#NAME?	C ₃₃ H ₃₉ N ₃ O ₄	541.688
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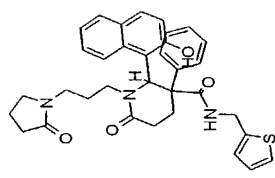
9100	660	1	000726043	9100-009	D 04	0 433	56.07	Spy4H	0 1776	TR0910000660	#NAME?	C ₃₂ H ₃₅ Cl ₂ N ₃ O ₃	580.552
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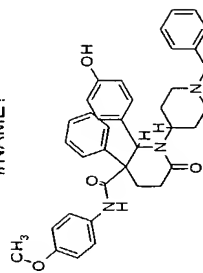
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc (mg/ml)	LionID	#NAME?	C ₃₅ H ₄₀ N ₄ O ₅	596.724
9100	3721	1	000728864	9100-051	A 07	0.298	55.80	Spy4H	0.1776	TR0910003721			



9100	3738	1	000728881	9100-051	B 09	0.275	55.80	Spy4H	0.1776	TR0910003738	#NAME?	C ₃₄ H ₃₅ N ₃ O ₄ S	581.734
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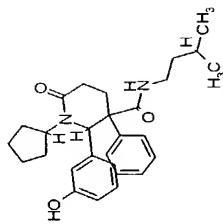


9100	2596	1	000727739	9100-037	D 06	0.263	55.71	Spy4H	0.1776	TR0910002596	#NAME?	C ₃₇ H ₃₉ N ₃ O ₄	589.732
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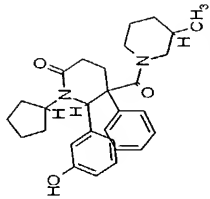


10091523 # 020322

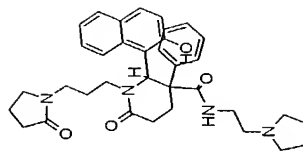
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?	C ₂₈ H ₃₅ N ₂ O ₃	448 603
9100	3221	1	000728364	9100-045	E 04	0.375	55.66	Spy4H	0.1776	TR0910003221				



9100	3235	1	000728378	9100-045	C 06	0.352	55.66	Spy4H	0.1776	TR0910003235		#NAME?	C ₂₉ H ₃₅ N ₂ O ₃	460 614
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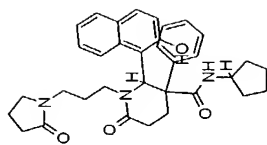
9100	3722	1	000728865	9100-051	B 07	0.26	55.50	Spy4H	0.1776	TR0910003722		#NAME?	C ₃₅ H ₄₂ N ₄ O ₄	582 741
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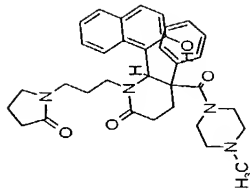
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?			
9100	702	1	000726085	9100-009	F 09	0.29	55.40	Spy4H	0.1776	TR0910000702	TR0910000702				

10991411991 # 00000000

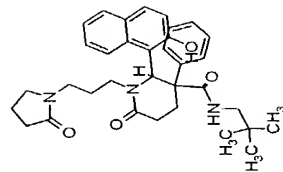
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C ₃₄ H ₃₅ N ₃ O ₄	553.699
9100	3725	1	000728868	9100-051	E 07	0.264	55.19	Spy4H	0.1776	TR0910003725			



9100	3729	1	000728872	9100-051	A 08	0.301	55.19	Spy4H	0.1776	TR0910003729	#NAME?	C ₃₄ H ₄₀ N ₄ O ₄	568.714
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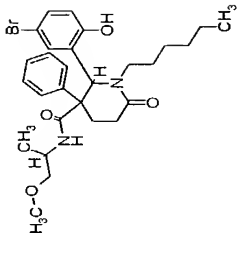
9100	3744	1	000728887	9100-051	H 09	0.268	55.19	Spy4H	0.1776	TR0910003744	#NAME?	C ₃₄ H ₄₁ N ₃ O ₄	555.715
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Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay Conc	mg/ml	LionID
9100	2473	1	000727616	9100-035	A 11	0.334	55.19	Spy4H	0.1776	TR0910002473

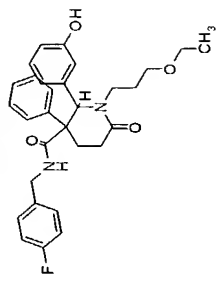
C₂₈ H₃₇ Br N₂ O₄ 545.514

#NAME?



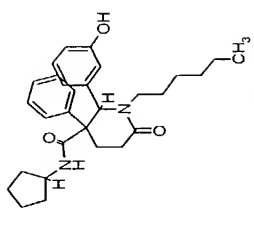
C₃₀ H₃₃ F N₂ O₄ 504.599

#NAME?



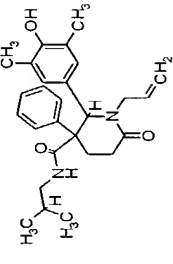
C₂₉ H₃₈ N₂ O₃ 462.63

#NAME?



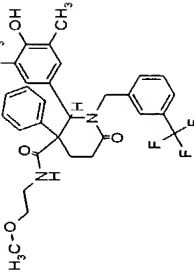
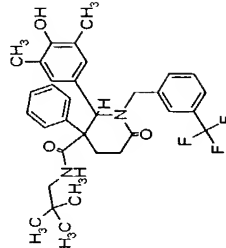
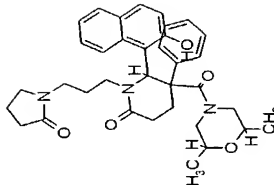
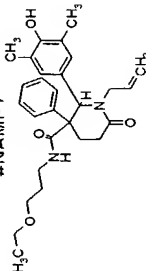
C₂₇ H₃₄ N₂ O₃ 434.577

#NAME?



40034505 : 000305

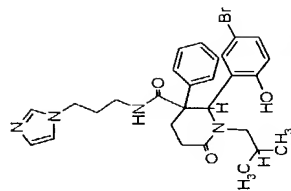
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	Chemical Structure	Formula	Mass
9100	863	1	000726246	9100-011	G 09	54.87	Spy4H	0.1776	0.487	TR0910000863	CHINA #NAME?		C ₃₃ H ₃₇ Cl N ₂ O ₃	545.119
9100	1052	1	000726435	9100-014	D 03	54.75	Spy4H	0.1776	0.419	TR0910001052	#NAME?		C ₃₀ H ₃₁ F N ₂ O ₃	486.584
9100	1077	1	000726460	9100-014	E 06	54.75	Spy4H	0.1776	0.257	TR0910001077	#NAME?		C ₂₃ H ₂₆ N ₂ O ₄	394.468
9100	206	1	000725589	9100-003	F 07	54.68	Spy4H	0.1776	0.305	TR0910000206	#NAME?		C ₂₄ H ₂₅ Br N ₂ O ₃	469.376
9100	2404	1	000727547	9100-035	D 02	54.55	Spy4H	0.1776	0.242	TR0910002404	#NAME?		C ₃₂ H ₃₄ N ₄ O ₃	522.646

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc (mg/ml)	LionID			
9100	687	1	000726070	9100-009	G 07	0.351	Spy4H	54.38	0.1776	TR0910000687	#NAME?		C ₃₁ H ₃₃ F ₃ N ₂ O ₄	554.606
9100	704	1	000726087	9100-009	H 09	0.399	Spy4H	54.38	0.1776	TR0910000704	#NAME?		C ₃₃ H ₃₇ F ₃ N ₂ O ₃	566.66
9100	3758	1	000728901	9100-051	F 11	0.285	Spy4H	54.27	0.1776	TR0910003758	#NAME?		C ₃₅ H ₄₁ N ₃ O ₅	583.725
9100	1062	1	000726445	9100-014	F 04	0.258	Spy4H	54.18	0.1776	TR0910001062	#NAME?		C ₂₈ H ₃₆ N ₂ O ₄	464.602

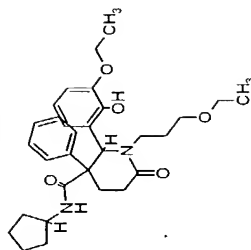
[illegible]

Library Compd Lot ExpReg Plate Well Raw Data Assay Result Assay Conc mg/ml LionID

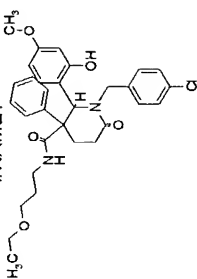
9100 1694 1 000726837 9100-023 F 03 0.304 54 15 Spy4H 0.1776 TR0910001694 #NAME? C₂₈ H₃₃ Br N₄ O₃ 553.498



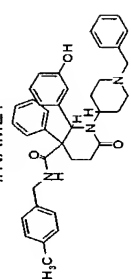
9100 2525 1 000727668 9100-036 E 07 0.325 54 11 Spy4H 0.1776 TR0910002525 #NAME? C₃₀ H₄₀ N₂ O₅ 508.655



9100 2742 1 000727885 9100-039 F 04 0.4 54.06 Spy4H 0.1776 TR0910002742 #NAME? C₃₁ H₃₅ Cl N₂ O₅ 551.08

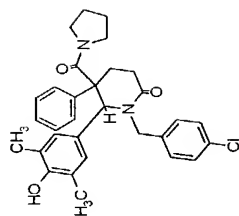


9100 2211 1 000727354 9100-031 C 08 0.323 54 05 Spy4H 0.1776 TR0910002211 #NAME? C₃₈ H₄₁ N₃ O₃ 587.76

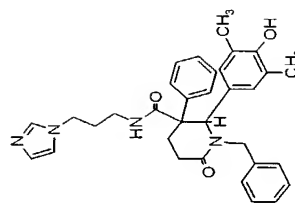


20071122 10:09:00

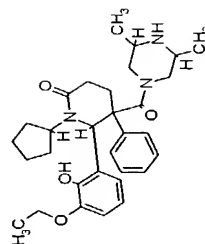
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C ₃₁ H ₃₃ Cl N ₂ O ₃	517.066
9100	2603	1	000727746	9100-037	C 07	0.467	53.70	Spy4H	0.1776	TR0910002603			



9100	2414	1	000727557	9100-035	F 03	0.258	53.59	Spy4H	0.1776	TR0910002414	#NAME?	C ₃₃ H ₃₆ N ₄ O ₃	536.672
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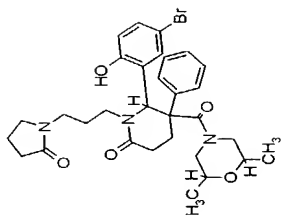


9100	1949	1	000727092	9100-028	E 05	0.281	53.49	Spy4H	0.1776	TR0910001949	#NAME?	C ₃₁ H ₄₁ N ₃ O ₄	519.682
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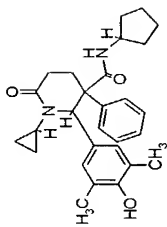


10001505 # 060200

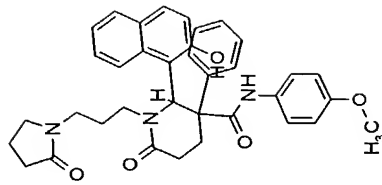
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc (ng/ml)	LionID	#NAME?	C ₃₁ H ₃₅ Br N ₃ O ₅	612.561
9100	998	1	000726381	9100-013	F 06	0.276	53.46	Spy4H	0.1776	TR0910000998			



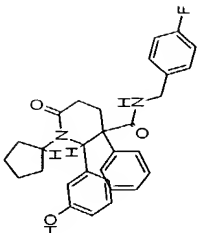
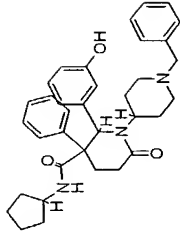
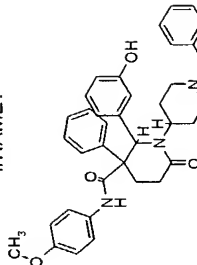
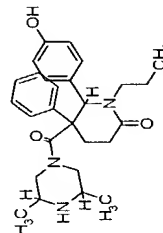
9100	765	1	000726148	9100-010	E 07	0.252	53.41	Spy4H	0.1776	TR0910000765	#NAME?	C ₂₈ H ₃₄ N ₂ O ₃	446.588
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9100	3756	1	000728899	9100-051	D 11	0.288	53.36	Spy4H	0.1776	TR0910003756		C ₃₆ H ₃₇ N ₃ O ₅	591.704
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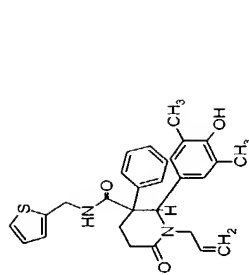


100944505 # 000303

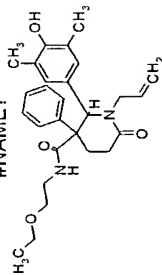
Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?	C ₃₀ H ₃₁ F N ₂ O ₃	486 584
9100	3213	1	000728356	9100-045	E-03	0.422	53.24	Spy4H	0 1776	TR0910003213				
9100	2205	1	000727348	9100-031	E 07	0.27	53.24	Spy4H	0 1776	TR0910002205			C ₃₅ H ₄₁ N ₃ O ₃	551.727
9100	2236	1	000727379	9100-031	D 11	0.276	53.24	Spy4H	0 1776	TR0910002236			C ₃₇ H ₃₉ N ₃ O ₄	589.732
9100	629	1	000726012	9100-008	E 10	0.258	53.22	Spy4H	0 1776	TR0910000629			C ₂₇ H ₃₅ N ₃ O ₃	449 591

486 584 551 727 589 732 449 591

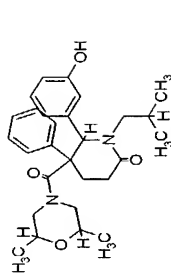
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C ₂₈ H ₃₀ N ₂ O ₃ S	474.622
9100	1058	1	000726441	9100-014	B 04	0.351	53.05	Spy4H	0.1776	TR0910001058			



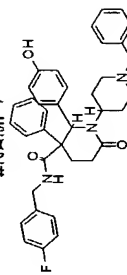
9100	1068	1	000726451	9100-014	D 05	0.261	53.05	Spy4H	0.1776	TR0910001068	#NAME?	C ₂₇ H ₃₄ N ₂ O ₄	450.576
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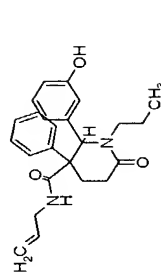
9100	598	1	000725981	9100-008	F 06	0.264	52.93	Spy4H	0.1776	TR0910000598	#NAME?	C ₂₈ H ₃₆ N ₂ O ₄	464.602
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9100	2573	1	000727716	9100-037	E 03	0.287	52.84	Spy4H	0.1776	TR0910002573	#NAME?	C ₃₇ H ₃₈ F N ₃ O ₃	591.723
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9100	1086	1	000726469	9100-014	F 07	0.263	52.76	Spy4H	0.1776	TR0910001086	#NAME?	C ₂₄ H ₂₈ N ₂ O ₃	392.496
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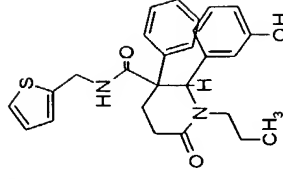


TR0910001058

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID
9100	1098	1	000726481	9100-014	B 09	0.298	52.76	Spy4H	0.1776	TR0910001098		

C₂₆ H₂₈ N₂ O₃ S

448.584

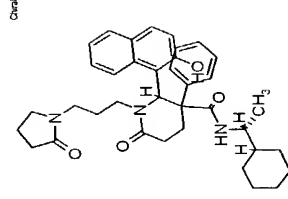


9100	3743	1	000728886	9100-051	G 09	0.347	52.75	Spy4H	0.1776	TR0910003743		
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C₃₇ H₄₅ N₃ O₄

595.779

#NAME?

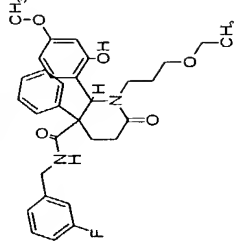


9100	812	1	000726195	9100-011	D 03	0.339	52.70	Spy4H	0.1776	TR0910000812		
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C₃₁ H₃₅ F N₂ O₅

534.625

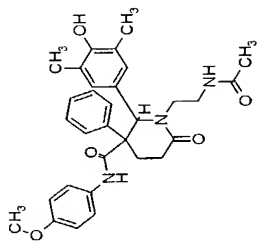
#NAME?



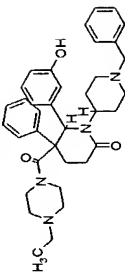
40934695 : 000000

Library	CrpId	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID
9100	2196	1	000727339	9100-031	D 06	52.69	Spy4H	0.1776	0.271	0.1776	0.271	TR0910002196

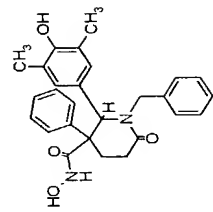
#NAME? C₃₁ H₃₅ N₃ O₅ 529 633



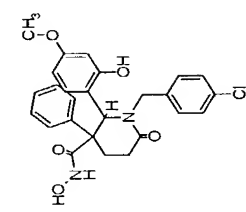
#NAME? C₃₆ H₄₄ N₄ O₃ 580 769



#NAME? C₂₇ H₂₈ N₂ O₄ 444 528



#NAME? C₂₆ H₂₅ Cl N₂ O₅ 480 945

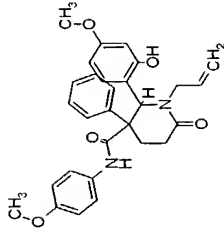


#634589 = 660307

Library	Compound	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc ng/ml	LionID
9100	2396	1	000727539	9100-033	D 11	0.334	52.60	Spv4H	0.1776	TR0910002396

#NAME?

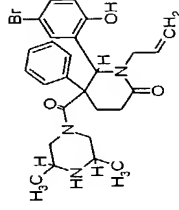
C₂₉ H₃₀ N₂ O₅ 486.565



9100	229	1	000725612	9100-003	E 10	0.266	52.55	Spv4H	0.1776	TR0910000229
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#NAME?

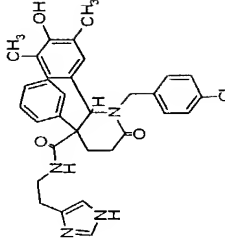
C₂₇ H₃₂ Br N₃ O₃ 526.472



9100	2604	1	000727747	9100-037	D 07	0.267	52.55	Spv4H	0.1776	TR0910002604
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#NAME?

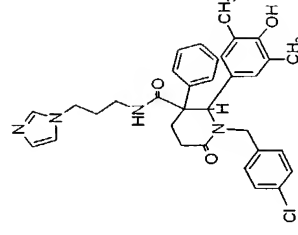
C₃₂ H₃₃ Cl N₄ O₃ 557.091



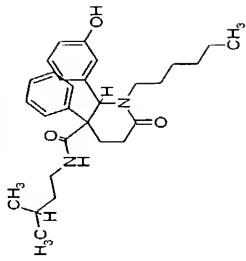
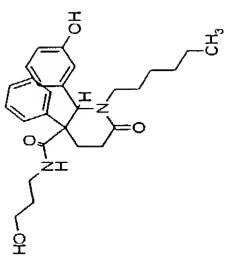
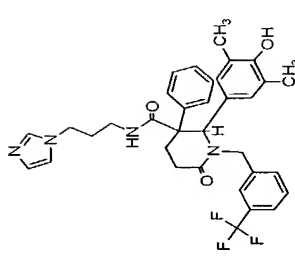
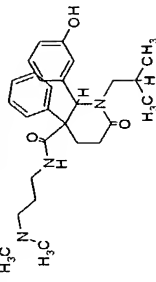
9100	2614	1	000727757	9100-037	F 08	0.317	52.55	Spv4H	0.1776	TR0910002614
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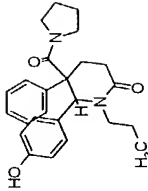
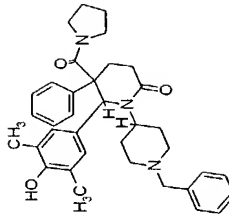
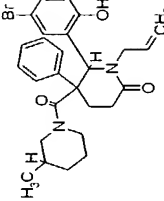
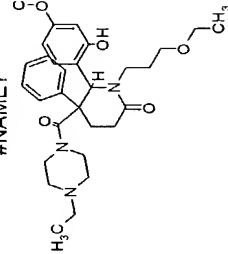
#NAME?

C₃₃ H₃₅ Cl N₄ O₃ 571.117



[illegible]

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C ₂₉ H ₄₀ N ₂ O ₃	464.646
9100	1021	1	000726404	9100-013	E 09	0.399	52.37	Spy4H	0.1776	TR0910001021			
9100	1027	1	000726410	9100-013	C 10	0.28	52.37	Spy4H	0.1776	TR0910001027		C ₂₇ H ₃₅ N ₂ O ₄	452.591
9100	694	1	000726077	9100-009	F 08	0.285	52.36	Spy4H	0.1776	TR0910000694		C ₃₄ H ₃₅ F ₃ N ₄ O ₃	604.669
9100	579	1	000725962	9100-008	C 04	0.261	52.35	Spy4H	0.1776	TR0910000579		C ₂₇ H ₃₇ N ₃ O ₃	451.607

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?				
9100	603	1	000725986	9100-008	C 07	0.269	52.35	Spy4H	0.1776	TR0910000603			C ₂₅ H ₃₀ N ₂ O ₃	406.523		
9100	4123	1	000729266	9100-057	C 07	0.289	52.30	Spy4H	0.1776	TR0910004123			C ₃₆ H ₄₃ N ₃ O ₃	565.754		
9100	235	1	000725618	9100-003	C 11	0.485	52.25	Spy4H	0.1776	TR0910000235			C ₂₇ H ₃₁ Br N ₂ O ₃	511.457		
9100	820	1	000726203	9100-011	D 04	0.272	52.16	Spy4H	0.1776	TR0910000820			C ₃₀ H ₄₁ N ₃ O ₅	523.67		

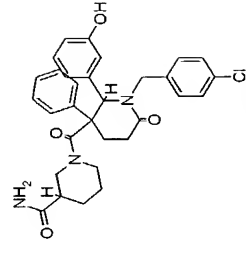
TR0910000603
TR0910004123
TR0910000235
TR0910000820

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID
9100	841	1	000726224	9100-011	A 07	0.354	52.16	Spy4H	0.1776	TR0910000841

#NAME?

C₃₁ H₃₂ Cl N₃ O₄

546.064

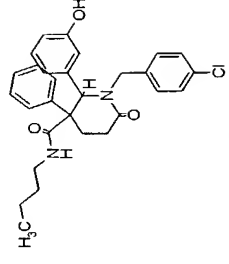


9100	872	1	000726255	9100-011	H 10	0.406	52.16	Spy4H	0.1776	TR0910000872
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#NAME?

C₂₉ H₃₁ Cl N₂ O₃

491.028

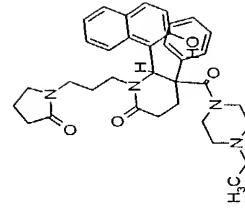


9100	3740	1	000728883	9100-051	D 09	0.275	52.14	Spy4H	0.1776	TR0910003740
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#NAME?

C₃₅ H₄₂ N₄ O₄

582.741

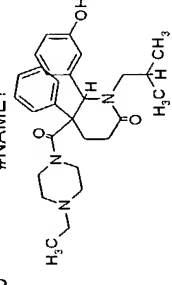


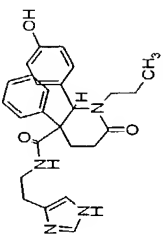
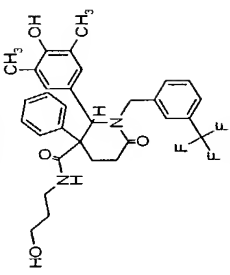
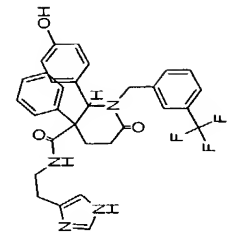
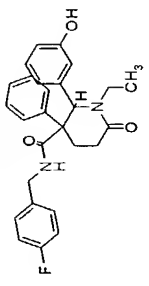
9100	580	1	000725963	9100-008	D 04	0.263	52.06	Spy4H	0.1776	TR0910000580
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#NAME?

C₂₈ H₃₇ N₃ O₃

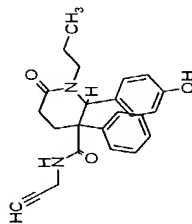
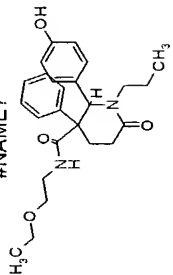
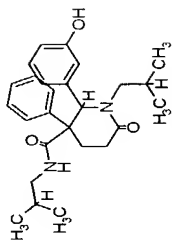
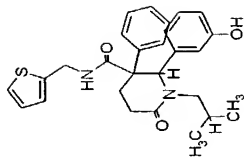
463.618



Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?			
9100	604	1	000725987	9100-008	D 07	0.261	Spy4H	52.06	Spy4H	0.1776	TR0910000604	C ₂₆ H ₃₀ N ₄ O ₃	446.548		
9100	707	1	000726090	9100-009	C 10	0.306	Spy4H	52.02	Spy4H	0.1776	TR0910000707	C ₃₁ H ₃₃ F ₃ N ₂ O ₄	554.606		
9100	4084	1	000729227	9100-057	D 02	0.264	Spy4H	52.02	Spy4H	0.1776	TR0910004084	C ₃₁ H ₂₉ F ₃ N ₄ O ₃	562.589		
9100	733	1	000726116	9100-010	E 03	0.253	Spy4H	51.92	Spy4H	0.1776	TR0910000733	C ₂₇ H ₂₇ F N ₂ O ₃	446.519		

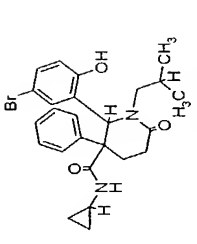
446.548 554.606 562.589 446.519

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc ng/ml	LionID	#NAME?				
9100	578	1	000725961	9100-008	B 04	0.334	51.77	Spy4H	0.1776	TR0910000578				C ₂₇ H ₃₀ N ₂ O ₃ S	462.611
9100	586	1	000725969	9100-008	B 05	0.301	51.77	Spy4H	0.1776	TR0910000586					
9100	628	1	000726011	9100-008	D 10	0.263	51.77	Spy4H	0.1776	TR0910000628					
9100	630	1	000726013	9100-008	F 10	0.264	51.77	Spy4H	0.1776	TR0910000630					

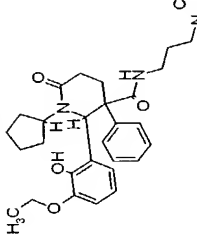


HOPELIFE = 000000

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc. mg/ml	Lioid	#NAME?	$C_{28}H_{28}Cl_2N_2O_4$	527.445
9100	2977	1	000728120	9100-042	A 04	0.341	51.75	Spy4H	0.1776	TR0910002977			

9100	1695	1	000726838	9100-023	G 03	0.442	51.74	Spy4H	0.1776	TR0910001695		$C_{25}H_{29}BrN_2O_3$	485.419
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9100	683	1	000726066	9100-009	C 07	0.546	51.69	Spy4H	0.1776	TR0910000683		$C_{32}H_{33}F_3N_2O_3$	550.618
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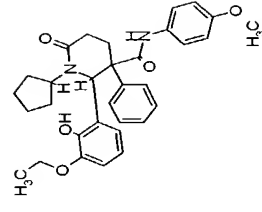
9100	1939	1	000727082	9100-028	C 04	0.287	51.58	Spy4H	0.1776	TR0910001939		$C_{30}H_{41}N_3O_4$	507.671
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Library Compd Lot ExtReg Plate Well Raw Data Assay Result Assay Conc mg/ml LionID
9100 1956 1 000727099 9100-028 D 06 0 29 51.58 Spy4H 0 1776 TR0910001956

C₃₂ H₃₆ N₂ O₅

#NAME?

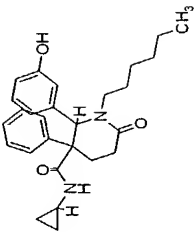
528.645



C₂₇ H₃₄ N₂ O₃

#NAME?

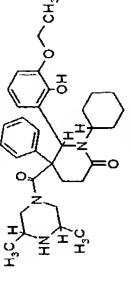
434.577



C₃₂ H₄₃ N₃ O₄

#NAME?

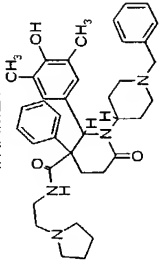
533.709



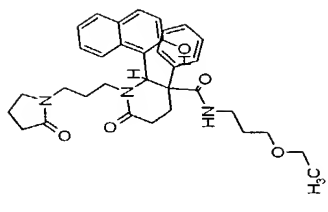
C₃₈ H₄₈ N₄ O₃

#NAME?

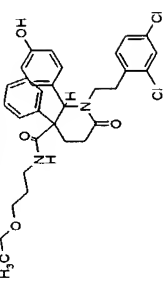
608.822



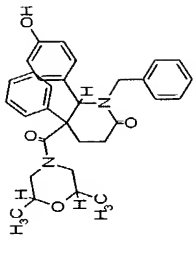
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?	C ₃₄ H ₄₁ N ₃ O ₅	571.714
9100	3742	1	000728885	9100-051	F 09	0.276	Spy4H	51.22	0.1776	0.1776	TR0910003742			



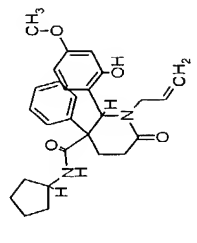
9100	2982	1	000728125	9100-042	F 04	0.438	Spy4H	51.21	0.1776	0.1776	TR0910002982	#NAME?	C ₃₁ H ₃₄ Cl ₂ N ₂ O ₄	569 526
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9100	1758	1	000726901	9100-023	F 11	0.298	Spy4H	51.20	0.1776	0.1776	TR0910001758	#NAME?	C ₃₁ H ₃₄ N ₂ O ₄	498 62
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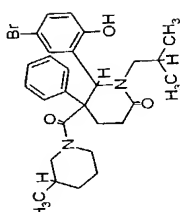
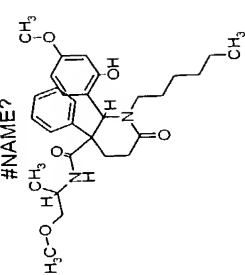
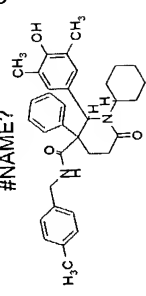
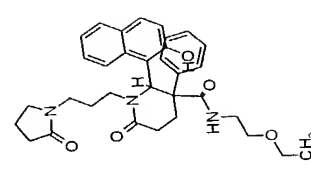


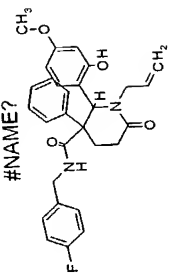
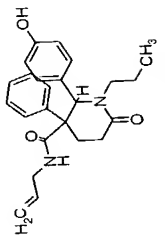
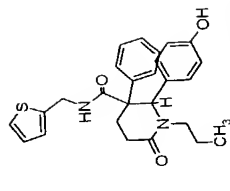
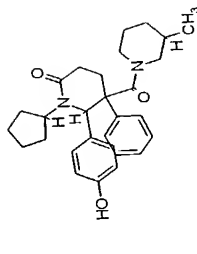
9100	2365	1	000727508	9100-033	E 07	0.34	Spy4H	51.19	0.1776	0.1776	TR0910002365	#NAME?	C ₂₇ H ₃₂ N ₂ O ₄	448.56
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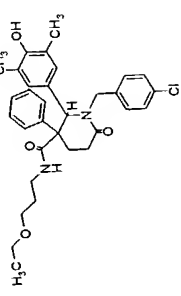


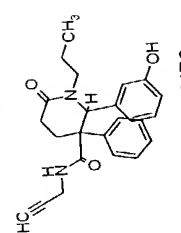
Library	Compound	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc ng/ml	LionID	
9100	2413	1	000727556	9100-035	E 03	0.49	Spy4H	51.02	0.1776	0.1776	TR0910002413	
												<chem>Cc1cc(O)c(C)cc1C(=O)Nc1ccc(F)cc1</chem>
												#NAME?
												C ₂₄ H ₃₃ F N ₂ O ₃
												536.644
9100	2466	1	000727609	9100-035	B 10	0.394	Spy4H	51.02	0.1776	0.1776	TR0910002466	
												#NAME?
												C ₂₈ H ₃₇ Br N ₂ O ₃
												529.515
9100	965	1	000726348	9100-013	E 02	0.337	Spy4H	51.02	0.1776	0.1776	TR0910000965	
												#NAME?
												C ₃₀ H ₃₆ Br N ₃ O ₄
												582.535
9100	1697	1	000726840	9100-023	A 04	0.363	Spy4H	50.94	0.1776	0.1776	TR0910001697	
												#NAME?
												C ₂₄ H ₂₉ Br N ₂ O ₄
												489.407

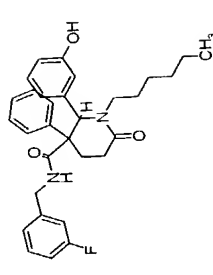
TR0910002413

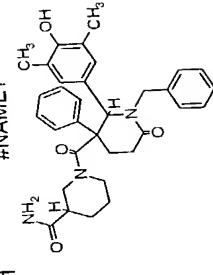
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C ₂₈ H ₃₅ Br N ₂ O ₃	527.5
9100	1715	1	000726858	9100-023	C 06	0.557	50.94	Spy4H	0.1776	TR0910001715			
9100	3033	1	000728176	9100-042	A 11	0.445	50.94	Spy4H	0.1776	TR0910003033		496.644	
9100	3691	1	000728834	9100-051	C 03	0.457	50.92	Spy4H	0.1776	TR0910003691		524.701	
9100	3748	1	000728891	9100-051	D 10	0.275	50.92	Spy4H	0.1776	TR0910003748		557.687	

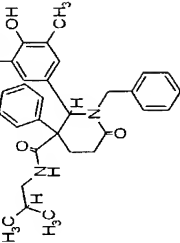
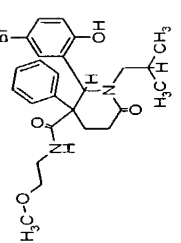
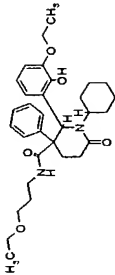
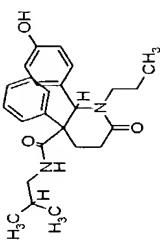
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID		
9100	2373	1	000727516	9100-033	E 08	0.351	50.91	Spy4H	0.1776	TR0910002373		C ₂₉ H ₂₉ F N ₂ O ₄ 488.556
9100	606	1	000725989	9100-008	F 07	0.266	50.90	Spy4H	0.1776	TR0910000606		C ₂₄ H ₂₈ N ₂ O ₃ 392.496
9100	618	1	000726001	9100-008	B 09	0.291	50.90	Spy4H	0.1776	TR0910000618		C ₂₈ H ₂₈ N ₂ O ₃ S 448.584
9100	2795	1	000727938	9100-039	C 11	0.392	50.87	Spy4H	0.1776	TR0910002795		C ₂₉ H ₃₅ N ₂ O ₃ 460.614

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc ng/ml	LionID	#NAME?	Chemical Structure	Molecular Formula	MW
9100	2622	1	000727765	9100-037	F 09	0.377	50.83	Spv4H	0.1776	TR0910002622			C ₃₂ H ₃₇ ClN ₂ O ₄	549.107

9100	1110	1	000726493	9100-014	F 10	0.272	50.78	Spv4H	0.1776	TR0910001110			C ₂₄ H ₂₆ N ₂ O ₃	390.48
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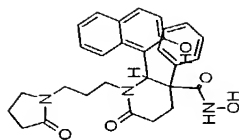
9100	1012	1	000726395	9100-013	D 08	0.517	50.75	Spv4H	0.1776	TR0910001012			C ₃₁ H ₃₅ FN ₂ O ₃	502.626
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9100	2401	1	000727544	9100-035	A 02	0.33	50.70	Spv4H	0.1776	TR0910002401			C ₃₃ H ₃₇ N ₃ O ₄	539.672
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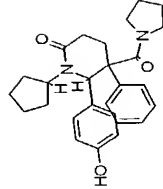
Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	Chemical Structure	Formula	Mass
9100	2426	1	000727569	9100-035	B 05	0.324	50.70	Spy4H	0.1776	TR0910002426	0.1776	TR0910002426	484.536		C ₃₁ H ₃₆ N ₂ O ₃	484.536
9100	1687	1	000726830	9100-023	G 02	0.338	50.67	Spy4H	0.1776	TR0910001687	0.1776	TR0910001687	503.434		C ₂₅ H ₃₁ Br N ₂ O ₄	503.434
9100	2342	1	000727485	9100-033	F 04	0.32	50.63	Spy4H	0.1776	TR0910002342	0.1776	TR0910002342	522.682		C ₃₁ H ₄₂ N ₂ O ₅	522.682
9100	626	1	000726009	9100-008	B 10	0.284	50.62	Spy4H	0.1776	TR0910000626	0.1776	TR0910000626	408.539		C ₂₅ H ₃₂ N ₂ O ₃	408.539

100727569 = 060206

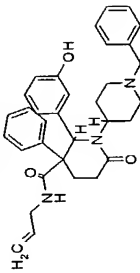
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	C ₂₉ H ₃₁ N ₃ O ₅	501.58
9100	3757	1	000728900	9100-051	E 11	0.272	50.61	Spy4H	0.1776	TR0910003757					



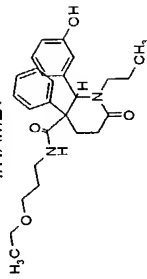
9100	2763	1	000727906	9100-039	C 07	0.322	50.58	Spy4H	0.1776	TR0910002763					
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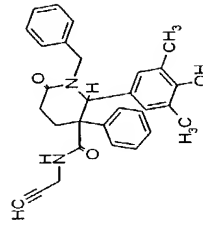
9100	2206	1	000727349	9100-031	F 07	0.277	50.51	Spy4H	0.1776	TR0910002206					
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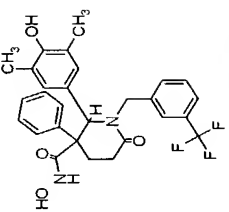
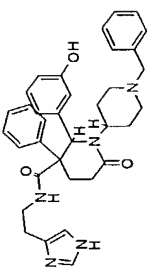
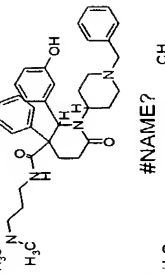
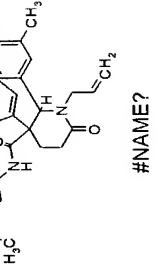
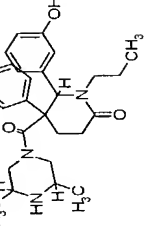


9100	1102	1	000726485	9100-014	F 09	0.271	50.50	Spy4H	0.1776	TR0910001102					
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9100	2430	1	000727573	9100-035	F 05	0.288	50.38	Spy4H	0.1776	TR0910002430					
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Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	C ₂₈ H ₂₇ F ₃ N ₂ O ₄	512.525
9100	717	1	000726100	9100-009	E 11	0.252	50.34	Spv4H	0.1776	TR0910000717					
9100	2204	1	000727347	9100-031	D 07	0.278	50.24	Spv4H	0.1776	TR0910002204				C ₃₅ H ₃₉ N ₅ O ₃	577.725
9100	2219	1	000727362	9100-031	C 09	0.282	50.24	Spv4H	0.1776	TR0910002219				C ₃₅ H ₄₄ N ₄ O ₃	568.758
9100	1059	1	000726442	9100-014	C 04	0.273	50.21	Spv4H	0.1776	TR0910001059				C ₂₈ H ₃₇ N ₃ O ₃	463.618
9100	1109	1	000726492	9100-014	E 10	0.273	50.21	Spv4H	0.1776	TR0910001109				C ₂₇ H ₃₅ N ₃ O ₃	449.591

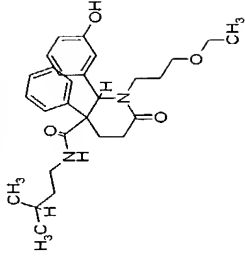
40994266 # 0209400

Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID
9100	1981	1	000727124	9100-028	E 09	0.283	50.21	Spy4H	0.1776	TR0910001981		

C₂₈ H₃₈ N₂ O₄

#NAME?

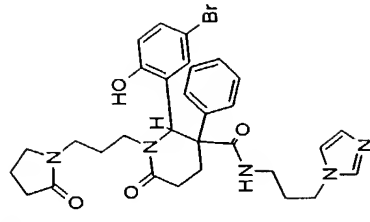
466.618



C₃₁ H₃₅ Br N₅ O₄

#NAME?

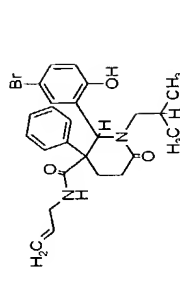
622.56



C₂₅ H₂₅ Br N₂ O₃

#NAME?

485.419



C₃₅ H₃₃ Cl₂ F N₂ O₃

#NAME?

619.561

